

Effects of Fuel Cell Material Properties on Water Management Using CFD Simulation and Neutron Imaging

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ABSTRACT

Effects of fuel cell material properties on water management were numerically investigated using Volume of Fluid (VOF) method in the FLUENT. The results show that the channel surface wettability is an important design variable for both serpentine and interdigitated flow channel configurations. In a serpentine air flow channel, hydrophilic surfaces could benefit the reactant transport to reaction sites by facilitating water transport along channel edges or on channel surfaces; however, the hydrophilic surfaces would also introduce significantly pressure drop as a penalty. For interdigitated air flow channel design, it is observable that liquid water exists only in the outlet channel; it is also observable that water distribution inside GDL is uneven due to the pressure distribution caused by interdigitated structure. An in-situ water measurement method, neutron imaging technique, was used to investigate the water behavior in a PEM fuel cell. The neutron imaging results of an operational PEM fuel shows that water content peak in the membrane was found close to catalyst layer for the low stoic case. The peak value increases with increasing current density and reaches its maximum at certain moderate current density then decreases due to heating effect at higher current density. Minimum water content can be observed inside GDLs, which is caused by the barriers from the hydrophobic nature of GDL pores. Finally, the PEMFC module in the FLUENT was used to build a PEM fuel cell model and preliminary model validation was performed using the previously obtained neutron results. It indicates that the current PEMFC module needs to be further improved to achieve better model predictabilities.

INTRODUCTION

For an operational fuel cell, the internal processes are very complicated. One issues pertaining to mass transfer loss and is critical for fuel cell design and optimization is water management [1]. Firstly, in an operating PEM fuel cell, in order to maintain high proton conductivity or lower proton transfer resistance, the polymer membrane must be under fully saturated conditions [2]. Secondly, excessive water in GDL and catalyst layer may cause flooding thus blocking reactants from reaching the reaction sites. In addition, the excessive water may introduce unbalanced water distribution inside a cell or in different cells of a stack, thus influencing the reactant transport and decreasing fuel cell performance. It is expected that significant performance gains and lifetime enhancement can be achieved with better understandings of water transport mechanism inside PEM fuel cells. Amongst various factors pertaining to performance of a unit cell or a fuel cell stack, material properties of fuel cell components play very important. Particularly, in terms of water management, properties closely related to water transport must be carefully considered in design and optimization. In this study, the effects of channel surface wettability on two-phase water transport were investigated using VOF model in the FLUENT. Both serpentine and interdigitated air flow channel configurations were studied. Next, neutron imaging techniques was adopted to investigate water transport in PEM fuel cell under steady state operating modes, and the results were used for preliminary validation of a PEMFC model. Finally, the conclusions were presented.

EFFECTS OF SURFACE WETTABILITY ON WATER BEHAVIOR IN REACTANT FLOW CHANNELS OF PEM FUEL CELL

In this section, VOF models in the FLUENT software with constant inlet boundary conditions will be applied to both serpentine and interdigitated reactant flow channel of a PEM fuel cell. The effects of channel surface wettability on water behavior, water content inside the channel, and two-phase pressure drop will be discussed in detail.

MODEL ASSUMPTIONS

To simplify the study, the following assumptions were invoked:

1. Isothermal condition - no temperature variation was considered in the simulations;
2. No detailed electrochemical mechanism considered. The computation domain of this model consists of air flow channel and GDL only, and we know that no reaction takes place in there, so the current problem could be simplified to a two-phase fluid mechanics problem with air flow and liquid water source applied on boundaries;
3. Product water generated through electrochemical reactions and the water transported from membrane are at liquid phase and the total water flux is assumed constant;
4. No water phase change is considered;
5. The GDL is modeled as homogenous porous media without considering detailed micro-structure.

COMPUTATIONAL METHODOLOGY

A commercial CFD software package, the FLUENT, was used to perform the simulations. Based on the conservation equations of mass and momentum, and a transport equation of volume fraction, the two-phase flow model can be used to conduct parametric studies on various material properties.

Liquid water and air were considered two immiscible fluids. Therefore the volume of fluid (VOF) model implemented in the FLUENT [3] can be adopted to capture the dynamic interface between them. In the VOF model, the basic continuity equation for the volume fraction, F , is solved first; then the reconstruction of the interface throughout the computation domain is performed in a post-processing fashion. For the i th phase, the volume fraction equation without considering source term and inter-phase terms has the following form:

$$\frac{\partial F_i}{\partial t} + \vec{v} \cdot \nabla(F_i) = 0 \quad (1)$$

The volume fraction for the primary phase (air in this case) can be computed based on the following constraint:

$$\sum_{i=1}^n F_i = 1 \quad (2)$$

The surface tension along the air-water interface and wall adhesion play important roles in a two-phase transport process in a micro-channel. In the FLUENT, a widely used surface tension model, the continuum surface force (CSF) model, proposed by Brackbill et al. [4] is adopted. With this model, the consideration of surface tension results in another portion of the source term in momentum equation, which is given as:

$$F_{\text{surface}} = \sigma_{ij} \frac{\rho_k \nabla F_i}{\frac{1}{2}(\rho_i + \rho_j)} \quad (3)$$

where σ_{ij} is the surface tension of the two phases (a constant air-water surface tension of 0.0662 N/m was adopted throughout this study) and K is the interface curvature. Additionally, effects of wall adhesion can be taken into account by specifying a wall adhesion angle (contact angle) in conjunction with the CSF model in the FLUENT.

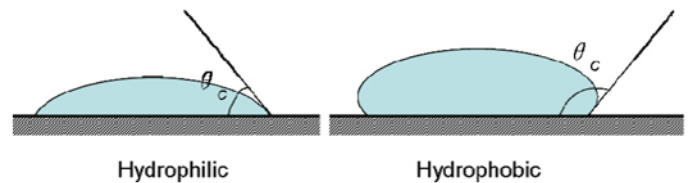


Figure 1. Contact angles and hydrophilic/hydrophobic surfaces

Surface wettability is also characterized by the contact angle [3]. Shown in Figure 1 is the definition of contact angle and two categories of surfaces - hydrophilic surface (contact angle less than 90°), and hydrophobic surface (contact angle greater than 90°). As an important parameter for bipolar plate design, contact angle must be optimized (for actual applications, various contact angles can be implemented through various surface coating techniques) to achieve effective water management.

EFFECTS OF SURFACE WETTABILITY ON WATER BEHAVIOR IN SERPENTINE REACTANT FLOW CHANNEL

Physical and Computation Domain

As shown in Figure 2, a U-shaped air flow channel (1 mm × 0.5 mm × 23 mm) was attached to a layer of porous media (GDL, such as carbon paper) of 0.2 mm thickness. This computation domain can be considered as a basic assembly element isolated from a complex gas flow channel configuration. Thus the information obtained from this simulation would provide useful insights to design and optimization of large scale bipolar plate as well.

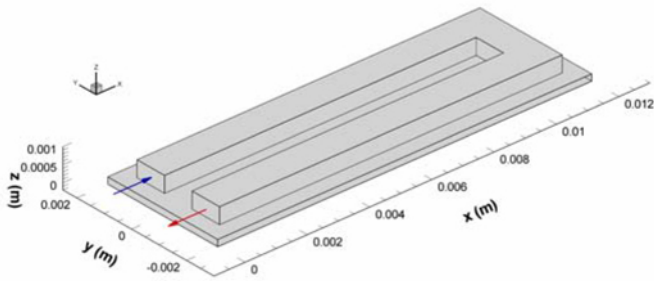


Figure 2. Computation domain: a U-shaped gas flow channel attached to a porous GDL

Boundary Conditions

For this 3-D two-phase flow simulation, no-slip boundary condition was applied to all the three interior walls of the channel. The wall adhesion effects can be taken into account by assigning different contact angles according to various channel material specifications. A velocity inlet boundary condition and an outlet boundary condition were applied at the channel inlet and outlet. The inlet air flow velocity was set to 1.43 m/s, corresponding to a PEM fuel cell operating at flow stoic ratio of 2, cell temperature of 80°C, and pressure of 2 atm.

On the bottom surface of the GDL, a constant liquid water mass flux boundary condition was applied. According to [5], the water flux at the GDL-catalyst layer interface can be modeled as:

$$N = \frac{M(1+2\alpha)i}{2F} \quad (4)$$

where M the molecular weight (18 g/mol for water), α the net water transport coefficient in the membrane (a constant of 0.1 in this study). i is the fuel cell operating current density (0.8 A/cm²) and F is the Faraday constant, 96,487 C/mol.

Evidently, the equation of water flux considers both oxygen reduction reaction and water transport from the membrane. The liquid water flux throughout the simulations was set to 0.0895 kg/s-m².

It should be pointed out that since the water generation rate of an operating PEM fuel cell is quite slow, the numerical value under the aforementioned operating condition (0.000895 kg/s-m²) was amplified by two orders of magnitude to shorten the water accumulation stage inside the GDL and facilitate the two-phase flow visualization inside the channel. In fact, for the quasi-steady state processes under consideration, the water distribution, water content inside the channel, and pressure drop are functions of channel geometry, channel surface wettability, and inlet air flow rate, as well as water generation rate. Considering the fact that the amount of liquid water inside the channel is quite small (as shown in the Results and Discussion section), the unrealities introduced by the amplified water generation rate are not significant.

Results and Discussions

The simulations in this study are capable of revealing unsteady features of the air-water flow in the channel. However, since in most of the time fuel cells operate under a relatively stable condition, the quasi-steady process characterized by the horizontal portion of Figure 3, where the water generation rate is balanced by the drainage rate out of the channel, is our focus throughout the simulation.

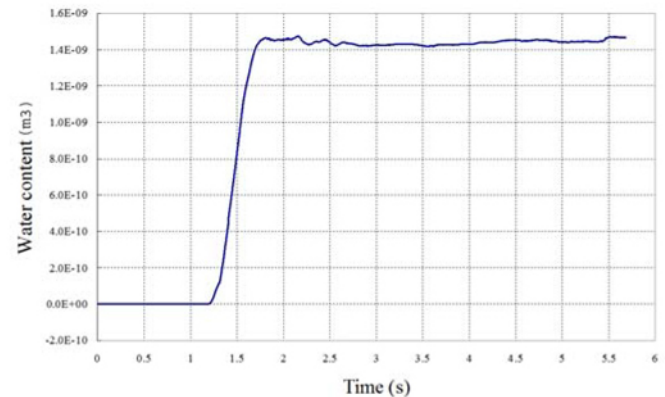


Figure 3. Water content in gas flow channel vs. time for a typical unsteady process

To investigate the effects of channel surface wettability on water management, five different contact angles were chosen to perform the parametric study. These cases were summarized in Table 1.

Table 1. Five simulation cases for the U-shaped channel with various surface wettabilities

Case #	Velocity (m/s)	Corresponding Inlet Air Reynolds number	Contact Angle (°)	Corresponding wettability
1	1.43	66	0	Hydrophilic (complete wetting)
2	1.43	66	45	Hydrophilic (partial wetting)
3*	1.43	66	90	N/A (no wall adhesion)
4	1.43	66	135	Hydrophobic (partial non-wetting)
5	1.43	66	180	Hydrophobic (negligible wetting)

* Baseline case for this study

Effects of Channel Surface Wettability on Water Behavior

By changing contact angles of the three channel surfaces, different water behaviors can be observed in the simulation results. For the baseline case (contact angle of 90°), a typical water distribution inside the channel is shown in [Figure 4](#), which shows the overall liquid water distribution. Ignoring the channel entrance, a liquid water film of nearly uniform thickness covers the whole GDL surface. The simulation results indicate that, at contact angle of 90°, water drainage takes place along the GDL surface and channel surfaces are of no help with water management. Obviously, this is not an optimal design.

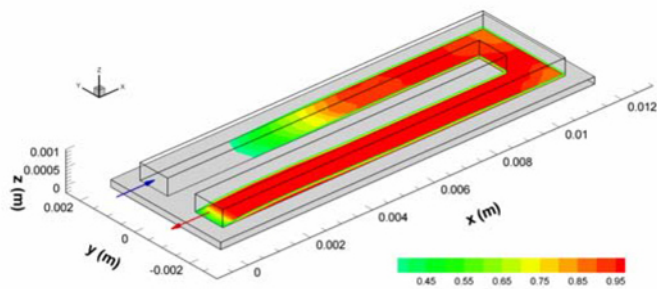


Figure 4. Liquid water distribution for the baseline case (1.43 m/s, 90 °)

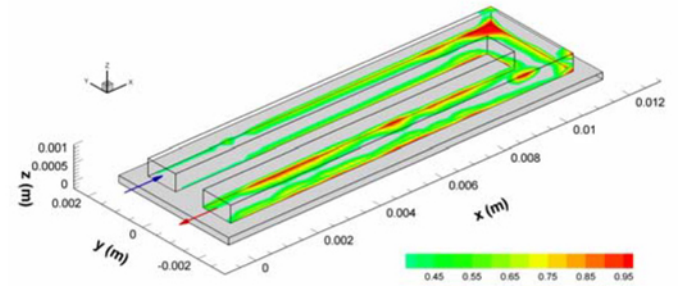


Figure 5. Liquid water distribution for case #2 (1.43 m/s, 45 °)

Now decreasing the contact angle to 45°, a partial wetting condition, the corresponding water distribution is given in [Figure 5](#). Compared with the baseline case, certain amount of water (droplets) is being removed through periodical corner flow along the outer upper edge. Along the lower edges, large amount of water removal is achieved through a continuous corner flow and it can be seen that this portion of water is prone to climbing up onto the side wall and spreading to form a larger contact area when flowing to the exit. This is due to the hydrophilic nature of the channel surfaces. In addition, the droplets grow in size when moving along the upper edge, by combining with the latish formed ones. These larger droplets cannot retain at their original location since the enlarged surface endures larger shear stress from air flow and the increased net force drags the enlarging droplets to the exit of the channel. Another point distinguishing from the baseline case is that the GDL surface area covered by water reduces significantly. In reality, the water film would be even smaller if the hydrophobic nature of the GDL surface were considered.

The liquid water behavior observed in case #2 can be qualitatively validated since it is quite consistent with some experimental observations published in open literature. For instance, in [6], liquid water distributions in air flow channel at different working conditions were captured by using a CCD camera and it was found that the liquid drop spreads on the channel sidewall and wicks into the corner - corner flow is an important water removal scheme when air velocity is low.

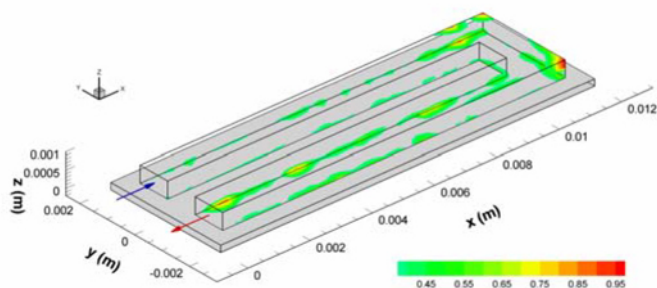


Figure 6. Liquid water distribution for the case #1 (1.43 m/s, 0°)

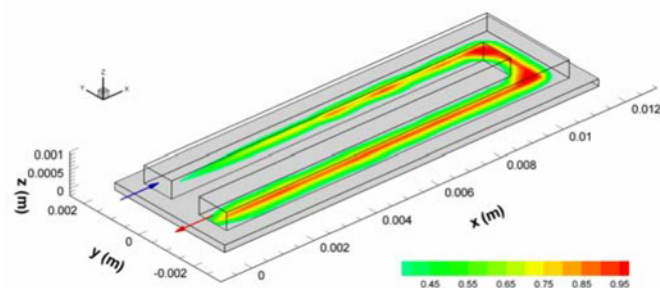


Figure 8. Liquid water distribution for case #5 (1.43 m/s, 180°)

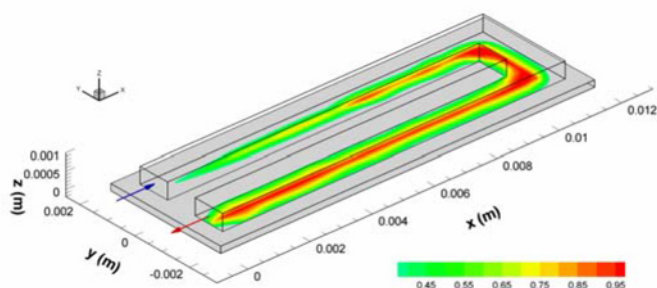


Figure 7. Liquid water distribution for case #4 (1.43 m/s, 135°)

What will happen in terms of water behavior if the channel surfaces are hydrophobic? Figure 7 and 8 are simulation results for the case of 135° and 180°, respectively. It is shown that in the case of using hydrophobic material, liquid water is prevented from touching the channel surfaces, resulting in almost no drainage flows along the channel walls. As a result, most of the GDL surface is covered by liquid water film with a parabolic cross-sectional shape, which forms a barrier to reactant transport to GDL. Obviously, this should be avoided in selecting and processing bipolar plate materials.

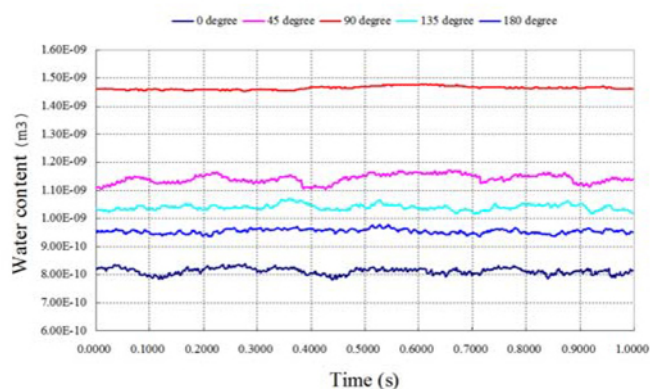


Figure 9. Water content history (inside the channel only) for all the five cases of various channel surface wettabilities

Please note that if the wettability and the detailed micro-structure of GDL surface were considered, additional information regarding water behavior would be available. For example, the droplet formation on the GDL surface may be observable at lower air velocity [7]; and a mist flow could be the flow regime for liquid water removal [6] at higher air velocity.

Effects of Surface Wettability on Water Content Inside the Channel

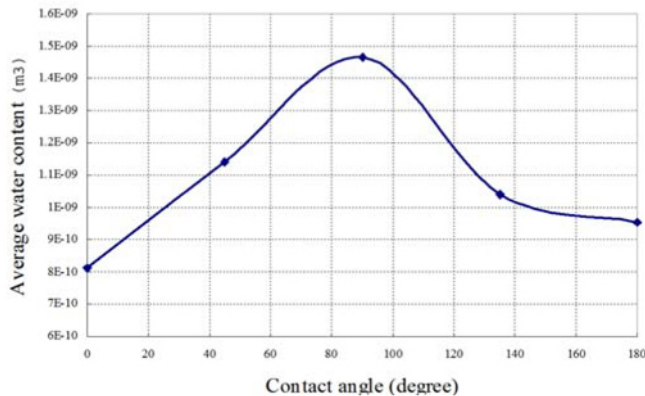


Figure 10. Average water content vs. contact angle

Figure 9 is the plot of water content history (inside the channel only) for all the five cases listed in Table 1. The water content inside the channel oscillates within a small range for each case. The most stable one is for contact angle of 90° but the water content is also the most. The water content values oscillate more significantly for all the other four cases, since the water transport in these cases is more active and periodic compared with the 90° case.

The plot of average water content vs. contact angle (Figure 10) indicates that, for the 90° case, it holds the most water, nearly twice the amount of the 180° case. An effective water removal strategy requires the water being removed as timely as possible and the water content in gas flow channels as less as possible. The material selection or manufacturing of bipolar plates should be away from the peak area as shown in Figure 10.

Effects of Surface Wettability on Pressure Drop Inside the Channel

A better understanding of the relationship between pressure drop and two-phase transport inside the gas flow channel is of importance for fuel cell system design because the two-phase flow characteristics in a micro-channel are significantly different from those of larger scales pipe flows [8]. The micro-channel or micro-pipe flow has been extensively studied since 1970's. Based on the simulation results obtained, discussions regarding pressure drop and surface contact angles are briefly presented in the following section.

Figure 11 shows the pressure drop history for the five cases with various surface wettabilities. A steady-state single-phase (air only) pressure drop line was added to the figure as well. Compared with the single phase case, the increase of pressure drop due to the introduction of liquid phase is quite significant. The increased pressure drop is attributed to (1)

the blockage effect due to added liquid water; and (2) wave drag effect introduced by the liquid water spreading on the channel wall surfaces. According to the simulation, the two-phase pressure drop should be in the range of 1.5 to 2.3 fold of its single phase counterpart.

It is also observable from Figure 12, plot of average two-phase pressure drop vs. contact angle, that for a hydrophilic channel surface the pressure drop decreases significantly as the contact angle increases. This is mainly due to the fact that the spreading area on the channel surface reduces rapidly with increasing contact angles, thus weakening the wave drag effect, as shown in Figure 5 and 6. In other words, the larger contact angle, the smaller water spreading area on the channel surface, thus the smaller drag force (interfacial tension) would exert on the gas flow, resulting in a decreased pressure drop. However, when the channel surface becomes more hydrophobic (contact angle greater than 90°), the pressure drop becomes much more constant. This attributes to the fact that, when the contact angle is greater than 90°, liquid water is pushed away from channel surfaces, forming a liquid film on the GDL surface; This liquid film is quite stable, and provides less contact area with the air flow, as shown in Figure 4, 7, and 8. We conclude that a hydrophilic channel surface is preferable, but it would induce a significant pressure drop inevitably.

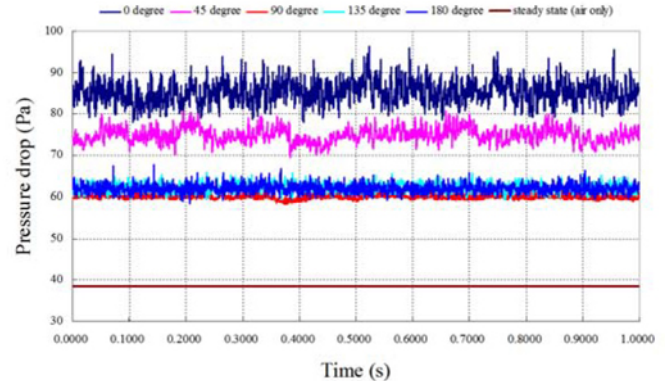


Figure 11. Two-phase pressure drop along the channel for all five cases with various channel surface wettabilities