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Residence time of water film and slug flow features in fuel cell gas channels and their effect on instantaneous area coverage ratio

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HIGHLIGHTS

- Liquid water removal mechanisms in PEM fuel cells are simulated with the VOF model.
- Slug flow and film flow conditions are assessed for different operating conditions.
- A hydrophilic range for the channel walls is proposed for enhanced water management.
- Liquid removal rate is balanced against GDL water coverage and two-phase pressure drop.
- An alternative trapezoidal channel cross-section shape enhances top wall film flow.

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ABSTRACT

Water in the gas channels of a Proton Exchange Membrane Fuel Cell is modeled as slugs and film, and removal mechanisms for these flow patterns are numerically investigated. The removal of excess liquid water is simulated using computational fluid dynamics (CFD) through the volume of fluid (VOF) model. The computational domain consists of a gas flow channel appropriate for commercial stacks for automotive applications. The effects of superficial air velocity, channel surface wettability, and channel cross-section geometry are investigated through quantitative comparison of two-phase pressure drop, area coverage ratio (ACR) over the gas diffusion layer (GDL) and liquid removal time. Top wall film flow was identified as a desirable feature since it did not cover the GDL and facilitated transport of oxygen to the reaction sites while removing the water. A range of hydrophilic channel walls in combination with a hydrophobic GDL is proposed to promote this behavior while reducing the fluctuations in two-phase pressure drop for different contact angles. Additional enhancements to liquid water removal were associated with the channel cross-section geometry. An alternative trapezoidal shape is suggested for improved top wall film flow while improving the manufacturability of the bipolar plates for mass production.

1. Introduction

Proton exchange membrane (PEM) fuel cells are electrochemical devices that have received significant attention due to their high energy conversion efficiency and clean operation at relatively low temperatures. These features, along with a high portability, make these devices an attractive option for both stationary and mobile applications. PEM fuel cells directly convert the chemical energy of hydrogen into electricity through an electrochemical reaction with oxygen, producing water as a by-product.

The most concerning issues preventing PEM fuel cells from global commercialization are those regarding the expensive fabrication materials (polymeric membrane and platinum in the catalyst layers) and the associated problems with the removal of the excess liquid water produced by the cell. In low temperature applications (e.g., automotive) liquid water may be accumulated in the gas flow channels due to the low saturation pressure of water in the system operating at temperatures ranging from the normal (25 °C) to freezing conditions. While a certain amount of water must be present in the polymer electrolyte membrane in order to promote

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its ionic conductivity, excess liquid water must be effectively removed from the gas diffusion layer (GDL) and the gas flow channels to prevent cell flooding and blockage of the reactant pathways.

The reactant streams supplied to the fuel cell are humidified with a certain amount of water in order to maintain the hydration level of the membrane; however, condensation of water from these streams and emergence of product water induce two-phase flow within the fuel cell. The flooding phenomenon may lead to mass transport limitations, causing cell voltage losses at high current densities [1] and voltage instabilities at low current densities [2].

Several experimental and numerical investigations are reported in the literature addressing the fundamentals of two-phase flow in PEM fuel cells [3–27]. Experimental visualization studies of the air/water two-phase flow in fuel cell channels have been conducted in operational fuel cells (in situ) [6–9], and in transparent microfluidic devices where liquid water is injected from external sources (ex situ) [10–16]. The main two-phase flow patterns that have been observed through these techniques at different operating conditions correspond to droplet flow, film flow, slug flow and mist flow.

Zhang et al. [7] experimentally investigated the liquid water transport in the channels of a transparent fuel cell for different operating conditions, reporting that top corner film flow is an efficient removal mechanism with a relatively low pressure drop. Sergi and Kandlikar [9] employed an in situ optical visualization setup for the quantification of the GDL water coverage with a video processing algorithm, comparing the two-phase flow patterns and cell performance for two different types of GDL. A modification of this algorithm was recently reported by Banerjee and Kandlikar [10] to obtain water coverage quantification data for different operating conditions simulated in an ex situ setup, focusing on equivalent current densities above 1 A cm^{-2}.

Bazylak et al. [13] investigated the dynamics of liquid water transport with an ex situ experimental setup, focusing on the emergence/detachment of droplets and breakthrough locations in the GDL. Lu et al. [14] employed a microfluidic ex situ device to identify the different types of two-phase flow regimes, where slug flow was observed predominantly at low airflow rates and associated it with severe flow maldistribution and performance degradation. The effects of channel surface wettability, cross-section geometry and orientation on liquid water removal were assessed in the study of Lu et al. [15]. They noted that hydrophilic gas channel walls provided a more uniform liquid distribution through film flow and a more stable pressure drop when compared to the hydrophobic case. Vertical orientation and a sinusoidal channel cross-section were also suggested for improved water management.

Although experimental visualization techniques provide qualitative estimation of how liquid water is transported in the flow channels, a clear identification of two-phase flow structures and quantification of important parameters such as water content and GDL water coverage ratio are limited. Computational fluid dynamics (CFD) modeling of multiphase flows is a powerful tool that offers the capability of a more detailed analysis of the liquid removal in PEM fuel cells.

The VOF model has been widely employed for the numerical simulation of droplet emergence, growth, deformation and detachment in the gas flow channels of PEM fuel cells [17–22]. Zhu et al. [17] analyzed the dynamic behavior of water droplets emerging from a pore into a straight microchannel using a three-dimensional VOF model. The effect of the cross-section geometry (rectangular, triangular, trapezoidal, and semi-circular, among others) on the removal of droplets was assessed for different wall surface treatments. The authors suggested a rectangular microchannel with an aspect ratio of 0.5, hydrophilic channel walls and a hydrophobic GDL in order to obtain a low flow resistance, low water hold-up, and low GDL water coverage.

Although droplet formation and emergence from GDL pores have been widely studied, liquid water builds up inside the channels due to multiple emergence points randomly located on the GDL that coalescence and eventually form films and slugs depending on the operating conditions. Only a few investigations have focused on the detailed analysis of film and slug flow structures. In an effort to investigate the slug formation and droplet accumulation in the gas flow channels of a PEM fuel cell, Carton et al. [23] employed the VOF method and compared their numerical results against water slug visualization in an ex situ test section with a double serpentine flow field. The formation of slugs was associated with channel blockage, depletion of the active area and therefore a decrease in performance. Quan and Lai [24] investigated the effects of surface wettability and airflow velocity on water removal from a single serpentine channel with sharped and curved corners. The results indicated that hydrophilic channel surfaces with sharp corners may provide an effective water removal mechanism, but at the expense of a higher pressure drop when compared to the hydrophobic case. The investigation of Le et al. [25] provided experimental validation of the VOF model for multiphase flows in simulating liquid water removal in PEM fuel cells, and demonstrated that hydrophilic channel walls may promote the formation of films at the channel corners. Ding et al. [26] simulated the transition of two-phase flow patterns in a straight channel with multiple pores at the GDL surface by increasing the liquid injection rate. Their results showed that the flow regime evolves from corner droplet flow to top wall film flow, followed by annular flow, and finally slug flow.

The use of hydrophilic channel walls for the enhancement of liquid water removal has been suggested by both experimental [7,15] and numerical studies [24,25,27]. However, the specific level of hydrophilicity and its effect on two-phase flow features of films and slugs has not been quantified or studied in detail yet. Ding et al. [27] coupled the VOF model with a 1D electrochemical model and investigated the effect of two-phase flow on PEM fuel cell performance by varying the liquid injection rates and surface wettability of the GDL and channel walls. Based on model predictions, the authors observed that hydrophobic channel walls increased the GDL water coverage ratio, hence reducing the cell output voltage. On the other hand, when using too hydrophilic channel walls (contact angle below 45°), the performance also decreased due to a longer liquid residence time. This indicates that there is a range of contact angles in the hydrophilic region that balances the liquid removal rate (associated to the surface tension component) with the GDL water coverage ratio.

The motivation of the present work is the detailed analysis of slug and film structures in order to find the optimum range of channel wall surface wettability and cross-section geometry for enhanced water management. The results will be qualitatively described by tracking the three-dimensional gas–liquid interface using the VOF model for different airflow velocities and channel dimensions. The removal features for the different configurations will be quantified by post-processing parameters such as two-phase pressure drop, water content and GDL water coverage ratio.

2. Computational model

2.1. Model assumptions

The following assumptions are made in the VOF model employed for the simulation of the two-phase flow in the gas channels:

1. Unsteady, laminar and incompressible flow.