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Numerical study of water management in the air flow channel of a PEM fuel cell cathode

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Abstract

The water management in the air flow channel of a proton exchange membrane (PEM) fuel cell cathode is numerically investigated using the FLUENT software package. By enabling the volume of fraction (VOF) model, the air–water two-phase flow can be simulated under different operating conditions. The effects of channel surface hydrophilicity, channel geometry, and air inlet velocity on water behavior, water content inside the channel, and two-phase pressure drop are discussed in detail. The results of the quasi-steady-state simulations show that: (1) the hydrophilicity of reactant flow channel surface is critical for water management in order to facilitate water transport along channel surfaces or edges; (2) hydrophilic surfaces also increase pressure drop due to liquid water spreading; (3) a sharp corner channel design could benefit water management because it facilitates water accumulation and provides paths for water transport along channel surface opposite to gas diffusion layer; (4) the two-phase pressure drop inside the air flow channel increases almost linearly with increasing air inlet velocity.

Keywords: Water management; PEM fuel cell; Air flow channel; Two-phase flow; Hydrophilicity; Pressure drop

1. Introduction

As one of the most promising technologies for auto transportation and power generation, proton exchange membrane (PEM) fuel cell has received great attentions from both academic institutions and industries due to its high efficiency, environmental friendliness, low working temperature, compact size, and rapid start-up feature. However, there remains much research and development work to make this energy conversion system more practical, durable, and economical for broader commercialization.

Water management is one of the critical issues for fuel cell design and optimization, and has been extensively studied both experimentally and numerically in the past decades. First of all, polymer membrane transferring the protons could only function well under fully saturated conditions in order to maintain good proton conductivity [1]. On the other hand, too much water may cause flooding at the electrodes thus blocking fuel and oxygen from reaching the reaction sites. In addition, excessive liquid water may also block the gas flow channel, or introduce unbalanced water distribution inside a cell or in different cells of a stack, thus affecting the reactant transport and decreasing the fuel cell performance. Water management inside gas flow channels can be optimized by reducing the liquid water coverage area on gas diffusion layer (GDL) surface, increasing drainage rate, minimizing pressure drop, etc. It is expected that significant performance gains and lifetime enhancement can be achieved with a better understanding of water transport phenomena inside PEM fuel cells.

For a single cell, water management could be considered in three sub-categories: water management in a proton exchange membrane, water management in gas diffusion layers, and water management in reactant flow channels. The first sub-category has been extensively studied since the beginning of 1990s and many numerical models regarding water management in membrane have been reported. The model proposed by Springer et al. [2] considered both electro-osmotic drag and diffusion of water through the membrane. They found that water transported through a membrane could be insignificant compared to the amount of water generated from the electrochemical reactions in a PEM fuel cell. In 1993, Nguyen and White [3] presented a steady, two-dimensional heat and mass transfer model for

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a PEM fuel cell. In this work, they considered liquid water transport through the membrane by electro-osmotic drag and diffusion and included the phase change of water. Recently, Cao and Djilali [4] studied the water management problem inside a membrane by applying conservation laws for water and current, in conjunction with an empirical relationship between electro-osmotic drag and water content, to obtain a transport equation for water molar concentration inside the membrane. The impacts of two-dimensionality, temperature, and pressure non-uniformities were analyzed and discussed.

Investigating water transport inside a porous GDL is not an easy task, neither by experiments nor by numerical simulations. So far, in situ experimental measurement of two-phase phenomena inside a porous GDL is still challenging and no detailed investigation was reported. In 2005, Litster et al. [5] conducted an ex situ visualization of liquid water transport in a PEM fuel cell GDL using fluorescence microscopy technique. In this experiment, fluorescein dye solution was pumped through the fibrous hydrophobic GDL and imaged with fluorescence microscopy. They found that liquid water transport through a porous GDL is only along a certain path, other than forming an "upside-down tree" capillary network. Neutron imaging and NMR microscopy techniques [6–13] seem very promising because of their non-intrusive nature and being capable of visualizing liquid water not only inside the gas flow channel but also in the porous GDL. In terms of numerical simulation, a GDL is usually mathematically described by using a porous media model, such as the work conducted by Li and Becker [14]. Essentially, a porous media model can be considered as a correction to the classical momentum conservation equation by adding a source term, which takes the effects of porous media on fluid flow into account. The drawback of using a porous media model is that the physically realistic pore structure cannot be considered explicitly.

Water management in gas flow channel is also very important. Bernardi and Verbrugge [15,16] and Springer et al. [2] investigated reactant transport through the GDL, but only vapor-phase water transport was considered in the gas flow channel. Recently, the study of water management in gas flow channel has been extended to two-phase. Zhang et al. [17] constructed a transparent single cell and by virtue of high-speed CCD camera, they observed the liquid water transport inside the gas flow channel and on the surface of the GDL as well. In this study, Liquid droplet formation and emergence from the GDL surface were characterized and liquid water removal mechanism from the GDL surface was identified. In addition, a theory was developed to determine what operating parameters and channel surface contact angles lead to sufficient liquid drainage from the fuel cell via corner flow. In 2005, Quan et al. [18] simulated the water behavior in a U-shaped air flow channel using volume of fraction (VOF) model in the FLUENT [19] computational fluid dynamics (CFD) package for the first time. In this work, five different cases with varying initial liquid water distribution were investigated. This work provided certain useful insights for understanding two-phase water behavior and introduced a new method for water management study in a PEM fuel cell. At the same time, Jiao et al. [20] did similar work for fuel cell stack with varying preset water distribution. Recently, Zhan et al. [21] conducted simulations to study droplet and film water motion in a flow channel of a PEM fuel cell using the same approach but the hydrophilicity of graphite plate and the hydrophobicity of the gas diffusion layer surface were taken into account. A common problem of all these works involving VOF model is that the liquid water must be placed a priori somewhere inside the computation domain, which makes the simulation less physically realistic and also makes the quasi-steady-state simulation, which provides important insight to the processes, unachievable.

In the following section, the model assumptions and formulations, boundary conditions, as well as the grid independency validation are summarized. Next, the effects of channel surface hydrophilicity, channel geometry, and air inlet velocity on water behavior, water content inside the channel, and two-phase pressure drop are discussed in detail. Finally, in Section 4, conclusions from the numerical study are drawn.

2. Numerical model and boundary conditions

2.1. Model assumptions

To simplify the study, the following assumptions were invoked:

(a) isothermal condition—no temperature variation was considered in the simulations;
(b) no detailed electrochemical mechanism considered. Since no reaction takes place in the gas flow channel and GDL, the current problem could be simplified to a two-phase fluid mechanics problem with air flow and liquid water source applied on boundaries;
(c) product water generated through electrochemical reactions and the water transported from membrane are at liquid phase and the total water flux is assumed constant;
(d) no water phase change is considered;
(e) the GDL is modeled as homogenous porous media without considering detailed pore structure.

2.2. Physical and computation domain

As one of the major aspects concerning water management, a simulation of water behavior inside an air flow channel would be incomplete without including the porous gas diffusion layer. In this study, as shown in Fig. 1, 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 understood as a basic assembly element isolated from a very complex gas flow channel configuration. Thus the information obtained from this simulation would provide useful insights for bipolar plate design and optimization.

2.3. Boundary conditions

For this 3D two-phase flow simulation, no-slip boundary condition was applied to all the three interior walls of the channel.