INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2017) 1–19

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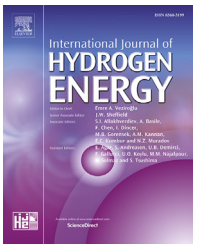

Increasing the performance of gas diffusion layer by insertion of small hydrophilic layer in proton-exchange membrane fuel cells

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ARTICLE INFO

Article history:
Received 17 July 2017
Received in revised form
25 November 2017
Accepted 4 December 2017
Available online xxx

Keywords:
Gas diffusion layer (GDL)
Wettability
Water saturation
Performance

ABSTRACT

The present study applied Lattice Boltzmann method (LBM) for examining the transport of liquid water in a GDL carbonic paper of polymer electrolyte membrane (PEM) fuel cells. The stochastic method is used for GDL carbonic paper reconstruction. In order to study the behavior of liquid water, different simulations are carried out on the reconstructed GDL. While removing from the GDL of a PEM fuel cell, the dynamics of liquid water is simulated by LBM in this study. The effects that the wettability of GDL imposes on the removal process and liquid water distribution are investigated. In addition, the dynamic behaviors and the saturation process of the liquid water in GDL in a steady state and a transient mode are also explored. The effects of surface wettability on the effective clusters in GDL, merging of different clusters and the loops developed by the fingers are investigated. Moreover, the effects of mixed wettability on the liquid water dynamic behavior and liquid water saturation within the GDL are studied in detail. The results show that the best location for insertion of the hydrophilic layer inside the GDL is near the GDL-GC interface. In this case, the time required for liquid water to reach the GDL/GC interface is reduced about 17% than purely hydrophobic GDL. A decrease of 18.7% in the steady-state saturation level is also observed by insertion of hydrophilic layer; therefore, use of hydrophilic layer near GDL-GC interface is more effective than increasing the contact angle of GDL-fibers. Different validation studies are also reported to show the accuracy of the model.

Introduction

Fuel cells serve as a conversion device. They somehow change the chemical energy of a fuel to the electrical energy using a process known as electrochemical reactions. It makes them more efficient than conventional heat engines [1]. The product of the reaction is usually water; thus, fuel cells are green and have extremely low emission. Considering the different technologies of fuel cells, polymer electrolyte membrane (PEM) fuel cells operate at lower temperatures. Therefore; PEM fuel cells have been pursued as the power source in wide range of engineering applications [2,3].

The flooding and dehydrations of a membrane is caused by the poor management in water resources of PEM fuel cells [4]. If excessive water accumulates in the components of a PEM fuel cells (i.e. gas channel (GC), gas diffusion layer (GDL), and catalyst layer (CL)), the problem of flooding is observed [5].

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https://doi.org/10.1016/j.ijhydene.2017.12.038

Flooding is a result of continuous generation of water in the cathode side without proper drainage [6]. Thus, the porous cathode of gas diffusion layer (GDL) is filled by liquid water as the flooding begins. In this condition; the effective transport of oxygen to the catalyst layer is hindered; leading to reactant starvation and performance loss [4]. On the other hand, membrane dehydration increases the proton conduction resistance and thus reduces the cell performance due to great ohmic loss across the membrane [5]. A key part of the water management in PEM fuel cells is liquid water transference in GDL [5]. GDL is considered important in the water management for striking the balance between the removal of water and membrane hydration [7]. Carbonic papers and carbonic cloths which are classifying as Porous carbon fiber structures, are mostly used for engineering GDLs. Carbon fibers used for fabrication of GDLs are hydrophilic and thus allow the accumulation of water within the pores of any engineered construct. As for facilitation of the gas and water's simultaneous transportation in reverse directions, polytetrafluoroethylene (PTFE) which is a non-wetting polymer is used in GDLs to give them hydrophobicity and to also reduce the construct's water saturation [5].

Liquid water transportation through a GDL is considered as a drainage process. In this process, the non-wetting liquid water displaces the wetting air. The displacement is dominated by capillary forces due to the low water flow rate and small pore sizes within the GDL as well as its high surface-area-to-volume ratio [5]. Under typical PEMFC operating conditions, the capillary number ($Ca = \mu u/\sigma$, in which μ is water dynamic viscosity, u serves as the velocity of liquid water, and σ is considered to be surface tension between water and air), which is the ratio measure between surface tension and viscosity forces, is of the order 10^{-6}–10^{-8} and the viscosity ratio M ($M = \mu_{water}/\mu_{air}$) is about 17.5, leading to capillary fingering in the GDL, considering the phase diagram that was proposed by Lenormand [8] for drainage flow.

Generally, the relationship between surface tension, viscosity, inertial and gravity forces are described by three pertinent dimensionless quantities including Ca, Weber number ((We), the correlation between inertial force and surface tension force, $We = \rho u^2 d/\sigma$) and Bond number (Bo, the correlation between gravity force and surface tension force, $Bo = (\Delta\rho)d^2g/\sigma$), μ shows water dynamic viscosity, u serves as liquid water velocity, σ is the tension of surface between water and air, d is the characteristic length, $\Delta\rho$ is the difference in density of water and air and g shows the gravity acceleration. In the cathode of PEM fuel cells, liquid water generating in the catalyst will enter GC after passing through the GDL [5]. In GDL of an operating PEMFC, *Ca* is of the order 10^{-6}–10^{-8}, *Bo* is about 10^{-9} and *We* is of the order 10^{-10} [9], indicating the dominance of surface tension on the liquid water transport in the GDL compared to the other forces [9].

Molaeimanesh and Akbari applied two-dimensional LB simulations to investigate the dynamics of water droplet when removing from the GDL of a PEM fuel cells in interdigitated flow field [1]. The results indicated that in the early stages when a droplet adhered to the MPL, its motion through a hydrophilic GDL caused creating different small droplets which were stuck to carbon fibers. So, it can also be said that droplet's motion is substantially facilitated by hydrophobic GDL.

Chen et al. investigated the dynamics and distributions of liquid water in GDL numerically [4] in the cases of with a land and without channel land. Their results showed a shorter time for transportation of liquid water from the inlet to the GC when hydrophilic channel land was considered. But more time was needed when the transportation occurred without channel land or with a hydrophobic channel land in the GC.

The transportation and distribution of liquid water in a gas diffusion layer (GDL) with porous structures was investigated by Chen et al. [5]. The GDL with microscopic porous structures was modeled using three dimensional reconstructions using the stochastic method. Simulation results showed that the transport mechanism of liquid water in the GDL was capillary fingering and liquid water pathway was interconnected, confirming the previous experimental results in literature. Further, effects of GC wettability were also explored and it was found that a hydrophilic GC leads to less liquid water accumulated in the GDL compared with a hydrophobic GC.

Mukherjee et al. showed the development of a mesoscopic modeling along with the realistic delineation of microstructures [9]. They wanted to show what effects the porous structures and also the wettability of surface will have on water transport and fluid dynamics in the PEFC catalyst layer and gas diffusion layer.

Hao and Cheng studied the wettability effect of dynamics of water transport in gas diffusion layer (GDL) [10]. They used a multi-phased free-energy lattice Boltzmann method (LBM) to simulate water invasion in a GDL which was filled initially by gas. It was proved that wettability was important in distribution of water saturation in a two-phase flow and in a GDL with uniform wettability.

Jeon and Kim studied the effects the compression ratio imposed on the dynamics of water transport in a GDL experimentally and numerically [11]. They visualized the liquid droplets growth in a channel for different compression ratios. It was showed that water advances through the channel with a small ratio of compression. Moreover, a large ratio of compression was estimated for the interface between the channel and rib.

Numerical studies of the interfacial effects on liquid water transport in porous materials in a PEM fuel cell is conducted using a two-phase lattice Boltzmann model by Han and Meng [12]. Numerical results clearly indicate that large perforated pores through the porous diffusion layers can serve as a convenient liquid water transport pathway and thus assist in liquid water removal. Results further show that an interconnected horizontal and vertical pore combination is especially beneficial to liquid water transport through the porous diffusion media in flooding conditions. Therefore, liquid water transport in the porous layers of a PEM fuel cell may be effectively managed through well engineered interfacial structures.

A 3D multiphase lattice Boltzmann model was established and employed to study the impact of PTFE content and distribution on the liquid-gas transport in PEMFC carbon-paper GDL by Chen and Jiang [13]. The 3D micro-pore structure of TGP-H-060 carbon paper was numerically reconstructed and part of the fibers' surface was randomly specified as PTFE. Two classes of cases were considered. One has PTFE uniformly distributed all through the GDL volume. The other has non-uniformly distributed PTFE. The simulation results about

Please cite this article in press as: Shakerinejad E, et al., Increasing the performance of gas diffusion layer by insertion of small hydrophilic layer in proton-exchange membrane fuel cells, International Journal of Hydrogen Energy (2017), https://doi.org/10.1016/j.ijhydene.2017.12.038