INTERFACIAL PHENOMENA AND HEAT TRANSFER IN PROTON EXCHANGE MEMBRANE FUEL CELLS

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Water transport and heat transfer are two critical issues for proton exchange membrane fuel cell (PEMFC) commercialization. Proper water and heat management ensure a sufficient reactant transport to reaction sites and high operating temperature, which requires good understanding of water and heat transport in PEMCs. In this paper, previous studies about interfacial phenomena related to water transport and heat transfer in PEMCs are reviewed. The interfacial phenomena in different components are discussed in detail. Experimental works have been conducted to visually observe the liquid water interface in PEMCs. However, difficulty still remains for investigations of interfacial phenomena. Modeling works on interfacial phenomena in PEMCs involve lattice Boltzmann, pore network, level set, and volume-of-fluid approaches. Different approaches have been applied for different components of PEMFC, and the liquid water interface can be located in all these approaches. Heat transfer in PEMCs is also introduced. Various heat sources result in diverse heat transfer phenomena and nonuniform temperature distribution in PEMCs. The components significantly influence heat transfer in PEMCs. Coupled heat and water transport is a major issue for PEMFC management, and the heat pipe effect has been identified as an important mechanism of coupled heat and water transport. Cooling is important for PEMFC heat management, especially for PEMCs with a large active area, high temperature, and stack.

KEY WORDS: review, proton exchange membrane fuel cell, interfacial phenomena, water transport, heat transfer

1. INTRODUCTION

The proton exchange membrane fuel cell (PEMFC) is an energy conversion device that converts the chemical energy of fuel directly into electrical energy by electrochemical reaction. Fig. 1 shows a schematic of a PEMFC. A typical PEMFC consists of a polymer electrolyte membrane sandwiched by an anode and a cathode. Both the anode and the cathode are composed of a catalyst layer (CL), gas diffusion layer (GDL), and bipolar plate with gas channel (GC).

Water is produced and heat is generated by the electrochemical reaction, which introduces the two most critical topics: water management and heat management in PEMCs. Excessive liquid water is known to accumulate in fuel cells, thereby resulting in severe flooding and deteriorating the performance of fuel cells. By contrast, a very low amount of liquid water will cause membrane dehydration, which affects the performance of fuel cells. Heat removal is important for membrane hydration. The generated heat will raise the operating temperature of PEMCs. If the operating temperature is too high, the membrane will dehydrate. Very low operating temperature is undesirable because of proton conductivity, electrochemical reaction kinetics, and water condensation. Thus, proper water and heat management are essential to ensure the operation stability and longevity of fuel cells.

Several review studies concerning water and heat management have been published by researchers (Siegel, 2008; Li et al., 2008; Bazylak, 2009; Das and Bansode, 2009; Ji and Wei, 2009; Kandlikar and Lu, 2009; Anderson et
al., 2010; Rosli et al., 2010; Jiao and Li, 2011; Tsushima and Hirai, 2011; Khan et al., 2011; Zhang and Kandlikar, 2012; Nasef and Aly, 2012; Kim and Lee, 2013; Ous and Arcoumanis, 2013; Kandlikar et al., 2014; Weber et al., 2014). These review studies discussed water management issues containing water transport, two-phase flow, water visualization, transport modeling, and water flooding, or heat management issues containing heat transfer and cooling techniques. For example, Weber et al. (2014) discussed the transport phenomena in PEMFC in the view of modeling. The basic equations used in models, multiphase flow, and catalyst layer modeling were analyzed.
Interfacial phenomena and heat transfer phenomena occur as water and heat undergo an electrochemical reaction. Liquid water emerges in the GDL to form a liquid–solid interface. Liquid water removed from the GCs will form a gas–liquid two-phase interface. Heat generated in the CL will transport to other components of PEMFCs and the reactants. Understanding these phenomena related to water and heat is important to properly manage water and heat in PEMFCs. This review focuses on interfacial phenomena and heat transfer in PEMFCs.

2. INTERFACIAL PHENOMENA IN PEMFCs

2.1 Interfacial Phenomena in the CL

Electrochemical reactions directly occur in the CL. Liquid water generates in the cathode catalyst layer (CCL). Initially, small water droplets form at the reaction sites and subsequently grow large. A portion of liquid water evaporates into the water vapor based on the operating temperature and saturation pressure. As reactants are supplied to the CCL to maintain the electrochemical reaction, multiphase phenomena will appear. Gas, liquid, and the CCL itself as a solid matrix coexist in the CCL, accompanied with an electrochemical reaction, which forms the most complex phenomena in the PEMFCs. Direct investigations of these phenomena are difficult because of the limitation of the PEMFC structure. Environmental scanning electron microscopy (ESEM) provides an option to observe the interfacial phenomena of water droplets in the CCL. Yu et al. (2005, 2006) and Nam et al. (2009) applied ESEM to observe the formation of liquid droplets in the CCL. Karsta et al. (2010) also observed liquid water on the surface of CCLs in fuel cells by scanning electron microscopy. The water droplet interface can be easily identified in the ESEM images. However, the observed CCL in their experiments is outside of an operating cell. In other words, these findings are ex situ experimental observations. Knowledge of the liquid water behavior in the CCL of an operating fuel cell is significant. Zhang et al. (2007) visually observed in situ water droplets on the CCL surface of an operating fuel cell. The evolution of liquid water on the CCL surface was presented. Many water droplets emerged at the beginning and then evaporated a few seconds later, depending on the location of droplets. More recently, Aoyama et al. (2014) observed ice at the interface between the CCL and microporous layer (MPL) in a frozen PEMFC. Although these studies are useful, experimental work on interfacial phenomena in the CCL is still lacking.

The investigation of interfacial phenomena in the CCL is experimentally intractable. Therefore, researchers have resorted to other attempts, such as the pore network (PN) method, lattice Boltzmann (LB) approach, or analytical solutions. Hannacha et al. (2011) obtained two-dimensional (2D) water invasion motion to analyze water transport in the CCL. In their PN, water invasion is controlled by capillary forces, which are the main driving forces for liquid water motion in the CCL. Based on the 2D PN, they proposed a three-dimensional (3D) PN to investigate the liquid water production mechanism in the CCL (Hannacha et al., 2012). The liquid water distribution in the CCL was obtained. An obvious pore-scale interface between the liquid phase and gas phase can be observed in the CCL PN models. Mukherjee et al. (2009) investigated liquid water transport in the reconstructed CL of a PEMFC by the LB method. The 2D phase distribution and 3D water distribution in the CL were obtained. To calibrate the two-phase LB model, the authors performed bubble and static droplet testing to evaluate the parameters related to interfacial phenomena, which are surface tension forces corresponding to fluid/fluid and wall adhesion forces corresponding to the fluid/solid. More details about the LB method in CL can be found in the literature (Mukherjee and Wang, 2006; Mukherjee and Wang, 2010; Mukherjee and Wang, 2011; Mukherjee et al., 2011). By deriving a one-dimensional analytical solution for liquid water transport through a CCL, Das et al. (2010) showed that CCL wettability significantly influences liquid water transport. A low contact angle or high wetting surface of the hydrophilic CCL can reduce the amount of liquid water.

The water or vapor produced may cover the reaction site in the CCL and block oxygen transport. Excessive liquid water even results in water flooding in the CCL. Apparently these occurrences have a negative effect on the performance of PEMFCs, which motivates the investigation of water behavior in CCLs. Based on the aforementioned literature, experimental works and modeling studies, including LB, PN, and theoretical analyses, are limited. In this review, more details about the LB and PN approaches are introduced in subsequent sections, in which several applications of LB and PN for the GDL exist.
2.2 Interfacial Phenomena in the GDL

2.2.1 Droplet Observation

The dominant driving forces for liquid water transport in the porous layer of PEMFCs are capillary forces. Thus, liquid water in the CCL is transported to the GDL because of capillary action. The water saturation is strongly related to capillary pressure, which can be supported by work of LaManna et al. (2014) on deducing the relationships of capillary pressure and saturation. If liquid water cannot be transported to the channel in time, water will accumulate at the void space in the GDL. Excessive accumulated liquid water will flood the GDL, which will block the gas transport pathway. Similar to the CCL, interfacial phenomena occur in the GDL. Direct observations of the interfacial phenomena in the GDL of fuel cells are difficult, even in a transparent fuel cell, because of the opaque GDL and its complex structures. Simplified experimental models have been developed to visually observe liquid water or liquid droplets in GDLs (Bazylak et al., 2008a; Gao et al., 2009; Liu and Pan, 2012). The emergence of discrete liquid droplets in the surface of GDLs is captured in these experiments. Evidence of discrete droplet emergence in GDLs has also been presented using ESEM (Nam and Kaviany 2003; Zhang et al., 2006). The growth, deformation, and breakthrough of a droplet occur on the surface of the GDL (Chen et al., 2005; Gao et al., 2009; Esposito et al., 2010a; Tan et al., 2011). Liquid droplets also show pinning behavior, which depends on the properties of the GDL (Bazylak et al., 2008a; Fishman et al., 2010). Preferential locations are chosen by droplets for breakthrough (Liu et al., 2012). Once droplet breakthrough occurs, the liquid water enters the channels. Afterward, the droplet grows into a slug at a low gas flow rate to block the channel (Hellstern et al., 2013; Wu et al., 2014).

Ex situ experiments have been conducted by Bazylak et al. (2008b) to show that the channel land hydrophobicity greatly affects the behavior of a droplet on the GDL surface. Moreover, Djilali and co-workers (Bazylak et al., 2008c; Litster et al., 2008) applied fluorescence microscopy to study the evolution of the gas–liquid interface inside a GDL through ex situ experiments. Although gas–liquid interfaces in GDLs can be visually observed in these ex situ experiments, such observations are not realized in a real operation fuel cell. Besides, X-ray radiography (Flückiger et al., 2011; Roth et al., 2013; Eller et al., 2014) and neutron radiography (Owejan et al., 2014) have been applied to visually observe water transport in GDLs. These observations are helpful, whereas water content or water saturation, not gas–liquid interface, was captured by these methods. Given this context, Eller et al. (2011) presented phase segmentation based on X-ray radiography. The segmentation of liquid and solid phases allows for quantitative analysis of liquid water in the GDL.

2.2.2 LB Approach

Given the difficulty in experimentally capturing the interface of a gas–liquid or liquid–solid in the GDL of fuel cells, simulation approaches provide a good option. An analytical model (Pasaogullari and Wang, 2004), numerical model (Polverino et al., 2013), mean value model (Esposito et al., 2010b), and full morphology (Schulz et al., 2007) have been applied to study water behavior in the GDLs. Meanwhile, considering the porous GDL in a micro perspective, pore level simulation approaches, such as the lattice Boltzmann method (LBM), are favored by researchers. Unlike conventional numerical simulations based on solving the mass, momentum, and energy equations, LBM simulates fluid flow or mass transport based on the Boltzmann equation at a mesoscopic level. As a mesoscopic approach, LBM can describe the gas–liquid two-phase flow in GDLs. Moreover, LBM can track the phase interface (Park and Li, 2008). It is a promising tool to detect water transport in GDLs by maintaining an obvious interface between the gas and liquid. Table 1 presents the studies that used LBM to investigate the two-phase flow with a distinct gas–liquid interface in the GDL and GC. LBM for GC application will be introduced in a subsequent section. The related interfacial phenomena and numerical details (e.g., computational size, dimension, validation, and other factors) are summarized. The related interfacial phenomena mainly focus on the behaviors of the liquid water (droplet) interface. A color is normally used to represent the liquid water phase, such as blue in Hao and Cheng (2010a) or red in Han and Meng (2013). Meanwhile, the gas phase is generally transparent in the literature. Thus, the interface is clearly identified. By contrast, Maggiolo et al. (2014) presented the liquid phase sites at the anode GDLs with different geometries. In addition, although LBM has been applied in several studies (Hao and Cheng, 2009a; Park et al., 2007) to investigate GDLs, no interfacial phenomena or obvious phase interfaces have been presented. Thus, they are not presented in Table 1.
## TABLE 1: Studies that investigated interfacial phenomena in GDLs and GCs of PEMFCs using LBM

<table>
<thead>
<tr>
<th>Reference</th>
<th>Related interfacial phenomena</th>
<th>Component</th>
<th>Computational domain size</th>
<th>Validation</th>
<th>Dimension</th>
<th>Wettability</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chen et al. (2012)</td>
<td>The behaviors of water droplet in GDL</td>
<td>GDL</td>
<td>2000 × 240</td>
<td>Convective-diffusive-reaction problem</td>
<td>2D</td>
<td>110°</td>
<td>SC model</td>
</tr>
<tr>
<td>Gao et al. (2013)</td>
<td>Water flow in hydrophobic/hydrophilic GDLs under different pressure drops</td>
<td>GDL</td>
<td>50 × 50 × 50</td>
<td>Simulation results compared with fitting</td>
<td>3D</td>
<td>Hydrophobic/hydrophilic</td>
<td>SC model</td>
</tr>
<tr>
<td>Han and Meng (2013)</td>
<td>Liquid water transport in GDLs with or without perforated pore</td>
<td>GDL</td>
<td>1000 × 400</td>
<td>Done in previous paper</td>
<td>2D</td>
<td>160°</td>
<td>BGK model cooperates with SC model</td>
</tr>
<tr>
<td>Hao and Cheng (2010a)</td>
<td>Water flow in GDLs with different contact angles</td>
<td>GDL</td>
<td>150 × 150 × 127</td>
<td>Nonwetting phase invasion through a perforated plate and two-phase displacement in a capillary channel</td>
<td>3D</td>
<td>92° or 115°</td>
<td>Free energy LBM</td>
</tr>
<tr>
<td>Kim et al. (2015)</td>
<td>Liquid water clusters in the GDLs</td>
<td>GDL</td>
<td>1000 × 400</td>
<td>Single-phase permeability calculation and two-phase droplet calculation</td>
<td>2D</td>
<td>100°, 120° or 140°</td>
<td>SC model</td>
</tr>
<tr>
<td>Koido et al. (2008)</td>
<td>Liquid water distribution in GDL with contact angles of 135° and 45°</td>
<td>GDL</td>
<td>122 × 122 × 122</td>
<td>--</td>
<td>3D</td>
<td>135° or 45°</td>
<td>SC model</td>
</tr>
<tr>
<td>Molaeimanesh and Akbari (2014a)</td>
<td>The removal process of a single droplet through GDLs having different untreated regions</td>
<td>GDL</td>
<td>3000 × 600</td>
<td>Drop test and static contact angle test</td>
<td>2D</td>
<td>Various contact angles</td>
<td>SC model</td>
</tr>
<tr>
<td>Molaeimanesh and Akbari (2014b)</td>
<td>The removal process of a single droplet initially adhering to MPL or the land through GDLs with uniform and nonuniform wettability</td>
<td>GDL</td>
<td>1024 × 250</td>
<td>Drop test and static contact angle test</td>
<td>2D</td>
<td>80° or 150°</td>
<td>SC model</td>
</tr>
<tr>
<td>Reference</td>
<td>Related interfacial phenomena</td>
<td>Component</td>
<td>Computational domain size</td>
<td>Validation</td>
<td>Dimension</td>
<td>Wettability</td>
<td>Model</td>
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<tr>
<td>Maggiolo et al. (2014)</td>
<td>Liquid phase site at the anode GDLs with different geometric parameters</td>
<td>GDL</td>
<td>–</td>
<td>Lattice Boltzmann EOS with results from reference</td>
<td>3D</td>
<td>90°</td>
<td>SC model</td>
</tr>
<tr>
<td>Niu et al. (2007)</td>
<td>Liquid water and gas flow under different pressure drops and contact angles</td>
<td>GDL</td>
<td>51 × 51 × 51</td>
<td>Static contact angle test</td>
<td>3D</td>
<td>105° or 120°</td>
<td>Free energy LBM</td>
</tr>
<tr>
<td>Park and Li (2008)</td>
<td>Droplet movement in GDL</td>
<td>GDL</td>
<td>150 × 150</td>
<td>Compared results with previous work</td>
<td>2D</td>
<td>–</td>
<td>BGK model</td>
</tr>
<tr>
<td>Tabe et al. (2009)</td>
<td>Water transport at different inflow velocities and capillary numbers; Behavior of liquid water and air flow in hydrophobic/hydrophilic GDLs</td>
<td>GDL</td>
<td>60 × 40</td>
<td>–</td>
<td>2D</td>
<td>150°</td>
<td>Free energy LBM</td>
</tr>
<tr>
<td>Zhou and Wu (2010)</td>
<td>Liquid water configuration under different conditions</td>
<td>GDL</td>
<td>2000 × 300 calculated from the GDL size and lattice spacing</td>
<td>Comparison with analytical results</td>
<td>2D</td>
<td>Mixed wettability</td>
<td>SC model</td>
</tr>
<tr>
<td>Amara and Nasrallah (2015)</td>
<td>The evolution of droplet interface</td>
<td>A micro-channel</td>
<td>150 × 40 \times 30</td>
<td>Comparing LBM results with the Laplace law</td>
<td>3D</td>
<td>Hydrophilic surface</td>
<td>SC model</td>
</tr>
<tr>
<td>Han and Meng (2012)</td>
<td>Droplet(s) behaviors in channels</td>
<td>Serpentine channels with round or sharp corner</td>
<td>500 × 300</td>
<td>Comparing the result of a single droplet emerging from micropore with the results in another study</td>
<td>2D</td>
<td>90°</td>
<td>BGK model cooperates with SC model</td>
</tr>
<tr>
<td>Han et al. (2012a)</td>
<td>The behaviors and interactions between water droplets emerging from two pores</td>
<td>A 500 μm-deep and 1000 μm-long channel</td>
<td>500 × 250</td>
<td>Comparing LBM results with the Laplace law and contact angle test</td>
<td>2D</td>
<td>GDL 120°</td>
<td>BGK model cooperates with SC model</td>
</tr>
<tr>
<td>Hao and Cheng (2009b)</td>
<td>The evolution of water droplet emerging from a micropore in channel bottom wall</td>
<td>A micro-channel</td>
<td>60 × 30 \times 120</td>
<td>Comparing LBM results with the Laplace law and contact angle test</td>
<td>3D</td>
<td>GDL: 110–170° Channel wall: 60°</td>
<td>Free energy LBM</td>
</tr>
</tbody>
</table>
One of the major parameters that affect the water transport process in GDL is the wettability of GDL, namely, hydrophilicity or hydrophobicity of the GDL. The concept of contact angle is normally used to characterize the hydrophilicity or hydrophobicity, which is the angle $\theta$ between the solid phase and gas–liquid or the interface of two fluids. Fig. 2(a) shows the schematic of contact angle between a water droplet and solid surface. If the contact

![Schematic of contact angle between a water droplet and solid surface.](image)

**FIG. 2:** The contact angle of a droplet on a solid surface: (a) Contact angle and (b) Receding and advancing contact angle.
the order of 10

describe the fluid flow in the pore and throat, researchers attempted to incorporate PN with the invasion percolation

PEMFCs. Pores and throats are used to reconstruct the GDL to form the pore space geometry morphology. To better
is a simplified pore space geometry morphology to simulate porous media with complex structures, such as GDL in

PN is another mesoscopic approach that can be used to investigate the interfacial phenomena in PEMFCs. A PN model

2.2.3 PN Approach

PN is another mesoscopic approach that can be used to investigate the interfacial phenomena in PEMFCs. A PN model

is a simplified pore space geometry morphology to simulate porous media with complex structures, such as GDL in

PEMFCs. Pores and throats are used to reconstruct the GDL to form the pore space geometry morphology. To better
describe the fluid flow in the pore and throat, researchers attempted to incorporate PN with the invasion percolation
algorithm (Cabellos and Prat, 2010; Wu et al., 2010a). In a typical operation fuel cell, the capillary number is of
the order of $10^{-8}$. Liquid water transport in porous media at such a low capillary number can be characterized as
capillary fingering, which is driven by the capillary force through the invasion percolation process. This capillary
fingering process has been confirmed as an important liquid water transport mechanism by many studies (Lee et al.,
2009a, 2010a, 2010b, 2012). Phase change including evaporation and condensation, which are the major sources
of water transport, also can be considered in PN models (Chapuis et al., 2008; Medici and Allen, 2013; Alink and
Gerteisen, 2013). In the invasion percolation process, the wetting phase is replaced by the nonwetting phase. For the
PEMFC application, the wetting and nonwetting phases represent the gas and liquid phases, respectively. Initially, the
pore and throat are filled with gas. Once the invasion process begins, liquid water starts to invade the pore or throat. A
pore or throat can be occupied by only one fluid. Thus, the liquid-gas phase interface can be automatically maintained.
Similar to LB, the interface is frequently distinguished by color. For example, the gas phase is transparent and the
liquid water phase is blue or another color. Table 2 presents the studies using the PN approach to investigate interfacial
phenomena in GDLs. The related interfacial phenomena, water sources, dimensions, and so on are summarized.

Interfacial Phenomena and Heat Transfer
### TABLE 2: Studies that investigated interfacial phenomena in GDLs using PN

<table>
<thead>
<tr>
<th>Reference</th>
<th>Wettability</th>
<th>GDL network size</th>
<th>GDL physical size</th>
<th>Dimension</th>
<th>Water sources</th>
<th>Related interfacial phenomena</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alink and Gerteisen (2013)</td>
<td>90°</td>
<td>–</td>
<td>220 × 1000 μm</td>
<td>2D</td>
<td>Liquid water injected from the bottom interface of GDL</td>
<td>Saturation distribution in GDLs</td>
</tr>
<tr>
<td>Chapuis et al. (2008)</td>
<td>Various contact angles</td>
<td>23 × 23</td>
<td>2.5 cm × 2.5 cm</td>
<td>2D</td>
<td>Constant water injection rate</td>
<td>Water invasion patterns in GDL</td>
</tr>
<tr>
<td>Hinebaugh and Bazylak (2010)</td>
<td>110°</td>
<td>60 × 30</td>
<td>800 × 400 μm</td>
<td>2D</td>
<td>Uniform water vapor flux from CL</td>
<td>Water breakthrough patterns in GDLs with the nucleation site</td>
</tr>
<tr>
<td>Ji et al. (2010)</td>
<td>Hydrophobic</td>
<td>–</td>
<td>300 × 300 × 200 μm</td>
<td>3D</td>
<td>Constant liquid flow rate at the inlet of MPL corresponding to 1 A cm⁻²</td>
<td>Liquid water clusters in GDL with time</td>
</tr>
<tr>
<td>Kang et al. (2008)</td>
<td>120°</td>
<td>–</td>
<td>30 cm × 30 cm × 7.2 cm</td>
<td>3D</td>
<td>Uniform water flux flow rate</td>
<td>Nonwetting fluid distribution</td>
</tr>
<tr>
<td>Kuttanikkad et al. (2011)</td>
<td>Mixed hydrophobicity (80° or 115°)</td>
<td>40 × 40 × 10</td>
<td>1080 × 1080 × 252 μm</td>
<td>3D</td>
<td>Liquid water reservoir with slow injection flow rate</td>
<td>2D water invasion patterns in GDLs with different fractions of hydrophobic pores</td>
</tr>
<tr>
<td>Lee et al. (2009a)</td>
<td>120°</td>
<td>20 × 20 × 10</td>
<td>400 × 400 × 200 μm</td>
<td>3D</td>
<td>Constant liquid water flow rate through inlet surface</td>
<td>Liquid–air interfaces formed during the liquid water transport in GDL</td>
</tr>
<tr>
<td>Lee et al. (2010a)</td>
<td>Hydrophobic</td>
<td>22 × 22 × 10</td>
<td>550 × 550 × 250 μ</td>
<td>3D</td>
<td>Uniform liquid water flux from pores at the inlet of GDL</td>
<td>Liquid water clusters; liquid water distribution with different boundary conditions</td>
</tr>
<tr>
<td>Lee et al. (2010b)</td>
<td>Hydrophobic</td>
<td>22 × 22 × 10</td>
<td>550 × 550 × 250 μ</td>
<td>3D</td>
<td>Uniform liquid water flux from pores at the bottom plane of GDL</td>
<td>Liquid water distribution in GDLs with or without pore paths</td>
</tr>
<tr>
<td>Lee et al. (2014)</td>
<td>120°</td>
<td>20 × 80 × 10</td>
<td>500 × 2000 × 250 μ</td>
<td>3D</td>
<td>Uniform liquid water flux at the bottom plane</td>
<td>Liquid water distribution in GDLs with different channel geometries</td>
</tr>
</tbody>
</table>
### TABLE 2: Continued

<table>
<thead>
<tr>
<th>Reference</th>
<th>Wettability</th>
<th>GDL network size</th>
<th>GDL physical size</th>
<th>Dimension</th>
<th>Water sources</th>
<th>Related interfacial phenomena</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medici and Allen (2010)</td>
<td>110°, 120°, 135°, 150°</td>
<td>120 × 12</td>
<td>3000 × 300 µm</td>
<td>2D</td>
<td>Water injected to the GDL with constant flow rate</td>
<td>Liquid water transport through GDLs</td>
</tr>
<tr>
<td>Medici and Allen (2013)</td>
<td>110°</td>
<td>120 × 12</td>
<td>3000 × 300 µm</td>
<td>2D</td>
<td>Uniform constant water flux</td>
<td>Water distribution in GDLs at different conditions</td>
</tr>
<tr>
<td>Nam and Kaviany (2003)</td>
<td>About 120°</td>
<td>10 × 10 (50)</td>
<td>–</td>
<td>2D</td>
<td>Water generated in vapor phase and then condensed into liquid water flowing to GDL</td>
<td>Water transport topologies</td>
</tr>
<tr>
<td>Shahraeeni and Hoofar (2014)</td>
<td>Mixed hydrophobic</td>
<td>15 × 15 × N N = (10, 17, 25, 33)</td>
<td>Only thickness (110, 190, 280, 370 µm)</td>
<td>3D</td>
<td>Constant water injection</td>
<td>The evolution of liquid water through GDLs</td>
</tr>
<tr>
<td>Sinha and Wang (2007)</td>
<td>110°</td>
<td>11 × 30 × 30</td>
<td>275 × 750 × 750 µm</td>
<td>3D</td>
<td>Liquid water reservoir at the inlet</td>
<td>Liquid water clusters in GDL</td>
</tr>
<tr>
<td>Sinha and Wang (2008)</td>
<td>60° – 120°</td>
<td>11 × 30 × 30</td>
<td>275 × 750 × 750 µm</td>
<td>3D</td>
<td>Liquid water reservoir connected to inlet</td>
<td>Liquid water distribution in GDLs</td>
</tr>
<tr>
<td>Wu et al. (2010b)</td>
<td>–</td>
<td>16 × 16 × 8</td>
<td>400 × 400 × 200 µm</td>
<td>3D</td>
<td>Liquid water reservoir with uniform pressure; Independent water injection point with uniform flux</td>
<td>Water distribution in GDLs with or without MPL</td>
</tr>
<tr>
<td>Wu et al. (2012a)</td>
<td>120°</td>
<td>20 × 20 × 10</td>
<td>500 × 500 × 250 µm</td>
<td>3D</td>
<td>Liquid reservoir</td>
<td>Liquid distributions in different slices of GDLs</td>
</tr>
<tr>
<td>Wu et al. (2012b)</td>
<td>Mixed wettability (80° or 110°)</td>
<td>80 × 80 × 12</td>
<td>2 mm × 2 mm × 300 µm</td>
<td>3D</td>
<td>Liquid water from CL to GDL through injection pore</td>
<td>Water distribution in different slices of GDLs with mixed wettability</td>
</tr>
<tr>
<td>Wu et al. (2013)</td>
<td>120°</td>
<td>40 × 40 × 12</td>
<td>1000 × 1000 × 300 µm</td>
<td>3D</td>
<td>Liquid reservoir</td>
<td>Liquid water distribution in different GDLs</td>
</tr>
<tr>
<td>Zhang et al. (2014)</td>
<td>Hydrophobic</td>
<td>–</td>
<td>–</td>
<td>3D</td>
<td>Water in CL</td>
<td>Water distribution in MPL</td>
</tr>
</tbody>
</table>

As a first attempt for PEMFC application, the PN GDL reconstructed by Nam and Kaviany (2003) consisted of randomly stacked carbon fiber, which may cause a highly disordered pore space topology. Possible water droplet
topologies in the reconstructed GDL were presented. Given the inherent nature of PN, the liquid water distribution or liquid water cluster has been presented in most other studies, such as the liquid water distribution in the model of Wu et al. (2010b). Thus, the interfacial phenomena in PN models are related to water transport. The MPL plays an important role in liquid water transport in PEMFC. The diffusion medium proposed by Nam and Kaviany (2003) to enhance the performance of PEMFCs is similar to the MPL. The MPL is capable of improving water management in PEMFCs. The existence of MPL reduces the liquid water content in GDLs (e.g., Kang et al., 2012), thereby alleviating water flooding. Wu et al. (2010b) presented the liquid water distributions under two different boundary conditions, with or without MPL. Although the liquid water distribution showed quite different patterns under these two boundary conditions, the MPL was revealed to reduce the liquid water content. This finding was consistent with the results from ex situ experiments (Lu et al. 2010a). Although the MPL has defects, such as cracks and holes, the consideration of cracks in the MPLs is a common phenomena, even in PN models (Medici and Allen, 2010; Ji et al., 2010; Wu et al., 2012a; Wu et al., 2013; Zhang et al., 2014). Liquid water prefers cracks in the MPL (Wu et al., 2012a; Zhang et al., 2014), so the introduction of cracks enables the MPL to function better. Although the MPL is beneficial to water management, how it affects liquid water transport remains unclear. Further research on the role of MPL is essential.

Boundary conditions are regarded as an important factor that influences the water distribution in the GDL. Two boundary conditions exist in the current PN models, namely, uniform water flux and uniform pressure. A detailed description of the boundary conditions can be found elsewhere (Wu et al., 2010b). Most PN models have applied either a uniform water flux boundary condition or a uniform pressure condition. Several works (Lee et al., 2009; Lee et al., 2010a; Wu et al., 2010b) applied two boundary conditions to investigate the effects of inlet boundary conditions. In an earlier attempt, Sinha and Wang (2007, 2008) applied a uniform pressure inlet boundary condition. However, as discussed in several studies (Lee et al., 2009a, 2010a), Lee et al. suggested that a uniform water flux boundary condition is more suitable to describe liquid water transport in the GDL of PEMFCs. The uniform pressure boundary condition causes nonuniform water flux at the inlet of the GDL surface, thereby deteriorating the performance of PEMFCs. Nevertheless, a uniform pressure boundary condition still has been adopted. Wu et al. (2012a) applied a uniform pressure boundary condition in their PN models to investigate the effects of MPL on mass transfer. The injection boundary condition significantly determines the water invasion patterns (Rebai and Prat, 2009). The liquid water distribution presented by Wu et al. (2010b) under two boundary conditions can be an evidence to prove it. Therefore, a reasonable water injection boundary condition that considers water generation and transport in PEMFCs is encouraged.

As discussed previously, wettability has an important effect on liquid water behavior. Rather than using hydrophobic GDLs to investigate the effect of wettability, Medici and Allen (2010), Sinha and Wang (2008), Kuttanikkad et al. (2011), and Wu et al. (2012b) adopted mixed wettability GDLs, which is more consistent with the practical GDL with PTFE treatment. The treated GDL performs better than the untreated GDL (Shahraeeni and Hoofar, 2014). Lee et al. (2009a, 2010a, 2010b, 2012) applied hydrophobic GDLs, and they incorporated a PN model with invasion percolation, which is prevalent in water behavior in hydrophobic GDLs. Chapuis et al. (2008) also suggested that applying hydrophobic GDL is a good option because liquid water saturation in a hydrophobic GDL is lower than that in a hydrophilic GDL. Previous mixed wettability investigations (Sinha and Wang, 2008; Kuttanikkad et al., 2011; Wu et al., 2012b) showed that the hydrophilic or hydrophobic fraction significantly affects the liquid water invasion patterns. Although an optimum GDL hydrophilic fraction exists (Sinha and Wang, 2008), its value is difficult to determine. Thus, the macroscopic treatment process is important, and more studies on the mixed wettability GDL are required.

### 2.3 Interfacial Phenomena in GC

#### 2.3.1 Two-Phase Flow Observation

When the liquid water generated in the CCL is transported to the GC, it will encounter the supplied gas, which leads to the formation of two-phase flow in the GC. The liquid water needs to be removed in time; otherwise, excessive liquid water accumulated in the GC causes severe water flooding, which greatly decreases the performance of a fuel cell. During drainage, the gas−liquid interface can be observed in the two-phase system. Tuber et al. (2003) was the
first group to apply a transparent fuel cell for water-flooding visualization. Since then, extensive works have been conducted on the two-phase flow visualization in the GC of an operating fuel cell. Even ice can be observed under frozen conditions (Biedof et al., 2014). Although visualization has also been conducted on the anode GC (Ge and Wang, 2007; Lee et al., 2009b; Sergi and Kandlikar, 2011; Lee and Bae, 2012), more attention has been paid to the cathode side because of the GC water-flooding problem, which is one of the main factors affecting the performance of fuel cells. Flooding is a persistent phenomenon in an operating PEMFC, which is greatly affected by various factors such as gravity (Kimball et al., 2008; Guo et al., 2009; Guo et al., 2014), GDL property (Spernjak et al., 2007; Jiao et al., 2010), and reactant flow rate (Weng et al., 2006, 2007; Dillet et al., 2010). New flow field designs (Metz et al., 2008) or a water absorption layer (Sugiuira et al., 2005) have been used to alleviate flooding. Applying a transparent window and high-speed video camera or similar instruments is a common method to observe the two-phase flow in the GC. In an operating fuel cell, the GC is in close contact with the end plate. The transparent window in the end plate enables a direct view of the GC, so the high-speed video camera or other instruments can record the two-phase flow. Fig. 4 presents visualized images of a serpentine flow field in the vertical and horizontal directions. The images were captured in our in situ experiments. The experiments were conducted under the following conditions: oxygen flow rate of 40 ml min$^{-1}$, hydrogen flow rate of 80 ml min$^{-1}$, and temperature of 50$^\circ$C. Droplets, slug, and mist are clearly observed, as shown in Figs. 3(a) and 3(b). Water droplets can be identified in the visualized images (Ma et al., 2006; Murahashi et al., 2008; Ous and Arcoumanis, 2009a, 2009b, 2009c). In addition to droplets, diverse flow patterns, including slug, film, and mist flow, can also be identified depending on the operating conditions (Zhang et al., 2006; Sergi et al., 2009). The images can be used as a tool to investigate the relation between voltage and flooding (Kim and Min, 2008; Cho et al., 2008; Masuda et al., 2008, 2011). The flooding area can be easily identified in the visualized images (Hakenjos et al., 2004). Hussaini and Wang (2009) used a liquid water cover area to present the flooding area because the water content is found to be quite constant under a given operating condition, but water distribution is different. The water distribution in channels has been proven to be nonuniform (Yang et al., 2004; Kandlikar et al. 2009; Anderson et al., 2011). Most studies merely observed the two-phase flow or flooding, without going into the concept of interfacial phenomena. Only a few involved the contact angle (Theodorakakos et al., 2006; Ous and Arcoumanis, 2009a; Zhan et al., 2012) or marking the gas–liquid interface (Liu et al., 2006, 2007, 2008). Except for the two-phase visualization in the GC of an operating fuel cell, numerous ex situ experiments have been conducted to observe two-phase flow. These experiments applied a simplified model to mimic the phenomena during an actual fuel cell operation process. Droplets (Ha et al., 2008; Lee et al., 2010; Colosqui et al., 2011; Venkatramana et al., 2009; Han et al., 2012b; David et al., 2012), together with slug, film, and mist flow patterns (Lu et al., 2009; Grimm et al., 2012; Wu and Djilali, 2012), can be obtained through ex situ experiments. Other patterns like annulus (Adroher and Wang, 2011) or intermittent and chaos flow (Chen, 2010), which are not the principal patterns in an operating PEMFC, can also be obtained through ex situ experiments. Slug flow occurs at low air flow rates, and film or mist flow appears at high flow rates. A droplet pattern may emerge at high flow rates as well. As shown in Figs. 4(a)–4(c), the slug in channels disappears with the increase in flow rates. Droplets and mist become the dominant pattern in the serpentine channels at higher flow rates, as shown in Fig. 4(c). The images in Fig. 4 were obtained from our in situ experiments. The experiments were conducted under various flow rates, and the temperature of the PEMFC was controlled at 60$^\circ$C. Apparently, air flow rate significantly affects the droplet behavior and two-phase flow. Besides, channel characteristics, including channel sidewall (Gopalan and Kandlikar, 2012, 2014), channel structure (Lee et al., 2011), and channel orientation (Lu et al., 2011), have important effects on the two-phase flow in the channel. Ex situ experiments allow the analysis of two-phase flow at certain operation conditions without the limitations of the fuel cell structure. Although the operation conditions similar to a real operating fuel cell can be acquired via artificial treatment, the phenomena are quite different from those in an actual fuel cell. In summary, the electrochemistry reaction is not considered in the ex situ experiments. These in situ and ex situ two-phase flow observations are helpful for fuel cell optimization. Shrivastava et al. (2015) measured ohmic resistance and current density by using a segmented cell. Only the anode was segmented, which showed a slight effect on hydrogen transport. The measurement of current density and ohmic resistance provides information to understand transport phenomena in the direction of land to channel. This may be a potential new technique to reveal local mass-transport limitations that affect the interfacial phenomena in PEMFCs such as two-phase flow in GCs. To better understand the interfacial phenomena in PEMFCs, a new technique should be introduced.
FIG. 3: Two phase flow in the serpentine channels of a PEMFC: (a) Vertical orientation and (b) Horizontal orientation.
FIG. 4: Two-phase flow in the cathode of PEMFCs operating at different flow rates: (a) Hydrogen: 60ml min-1, Oxygen: 30ml min-1, (b) Hydrogen: 80ml min-1, Oxygen: 40ml min-1, and (c) Hydrogen: 100ml min-1, Oxygen: 50ml min-1.

2.3.2 Level Set

The level set (LS) approach is based on the finite element method to solve governing equations, such as the continuity equation. It can accurately track the gas–liquid interface by the LS function $\phi$. The governing equations are solved using COMOSOL Multiphysics. The interface curvature, surface tension, and contact angle, which are parameters related to interfacial phenomena, can be considered in the LS model. To date, only a few researchers have applied the LS method to investigate droplet behavior in a simple GC (Mukherjee and Kandlikar, 2006; Choi and Son, 2008, 2009; Akhtar and Kerkhof, 2011). Given the spatial continuous distribution of the LS function, the interface curvature
and parameters related to interface curvature can be accurately calculated. Thus, the liquid droplet interfaces are explicitly presented in these studies to discuss droplet motion. Mukherjee and Kandlikar (2006) are the pioneers in this topic. They numerically analyzed the growth and departure of a liquid water droplet that was initially placed near the center of a straight channel top wall. A tapered channel was applied by Akhtar and Kerkhof (2011) to investigate the effect of wall property on water droplet dynamics. Choi and Son (2008, 2009) also studied the behavior of liquid water droplet(s) using the LS method. Application of the LS method in PEMFCs is limited, and most research focused on the droplet(s) initially positioned on the wall of the channel.

2.3.3 Volume of Fluid

The volume-of-fluid (VOF) approach is another numerical method that can trace the phase interface. In a VOF model, the phase interface is captured by determining the volume fraction for the fluids. In one fluid (e.g., liquid phase), the volume fraction is equal to 1. In another fluid (e.g., gas phase or another liquid phase), the volume fraction is equal to 0. The location with volume fraction between 0 and 1 is identified as the phase interface. Compared with the LS method, the VOF method involves a complicated calculation of phase interface construction. Accurately calculating the interface curvature and quantity related to interface curvature using this method is difficult. However, the phase interface construction enables the VOF method to capture a complex phase interface. Besides, the addition of surface tension and contact angle can be realized in a VOF model. More details about the VOF method can be found in the review study of Ferreira et al. (2015). The VOF method is favored by researchers to track the phase interface in gas–liquid two-phase flow. A large number of studies have been conducted on liquid water transport in the GC of PEMFCs using the VOF method. Table 3 presents the dimensions, component details, research subject, and interfacial phenomena of previous studies using the VOF method. VOF models (Suresh and Jayanti, 2010; Park et al., 2010; Ahmad et al., 2013; Yin et al., 2014) for liquid transport in GDLs have also been developed. These studies are listed in the last section of the Table 3.

As mentioned previously, liquid water emerges from the GDL surface as liquid droplets that transport into the GC. To simulate this scenario, the emergence of a single droplet in the GC is easy to implement. Two methods have been used in the present study to simulate a single droplet in the GC. The simplest approach is to initially place a single droplet in the GC. Quan et al. (2005) investigated droplet movement inside a U-shaped microchannel. Zhan et al. (2006) also adopted this method to investigate the motion of a single liquid droplet in straight and serpentine channels. The single droplet was initially located at the center of the channel. They found that a straight channel is more suitable for removing liquid water than the serpentine channel. However, the length of the channel is much shorter than that of an actual fuel cell, so the results do not completely reflect the actual characteristics of a droplet in a GC. Qin et al. (2013a, 2013b, 2014) detected the motions of a single droplet initially placed in a straight channel attached to the membrane electrode assembly (MEA) surface. A needle (Qin et al. 2013a, 2013b) and a plate (Qin et al. 2014) were inserted in the channel to accelerate the removal of the liquid droplet. Instead of focusing on droplet movement in the GC, Theodorakakos et al. (2006), as well as other researchers (Golpaygan and Ashgriz, 2005; Shirani and Masoomi, 2008; Fang et al., 2008; Golpaygan et al., 2011), paid more attention to droplet deformation. Several studies (Cai et al., 2006; Dupont et al., 2011; Mondal et al., 2011) emphasized the effect of surface wettability, which remarkably influences liquid water transport in GCs. Another approach for single droplet simulation is to simulate droplet emergence from the GDL at a certain velocity. Generally, a pore is positioned on the bottom wall of the channel where liquid water is injected. However, different pore locations result in diverse droplet behavior (Zhu et al., 2011; Bao et al., 2014). The initial processes of the droplet interface movement presented in studies are similar to some extent. At the beginning of simulation, a small liquid water droplet emerges from the pore. The droplet then becomes bigger and deformable because water is continuously injected through the pore. Afterward, the droplet detaches from the pore and moves along the channel. After detachment, the droplet exhibits relatively diverse behavior, depending on the operating conditions. The droplet behavior greatly depends on the operating conditions, such as air velocity (Zhu et al., 2008a; Chen et al., 2012b; Qin et al., 2012), wettability or contact angle (Zhu et al., 2008b; Minor et al., 2008), and channel geometry (Zhu et al., 2007, 2010). The property of GDL has also been proven to affect movement at the liquid water interface (Chen et al., 2012c, 2013). The majority of previous studies applied a typical single straight channel, which limits the valuable guidance for fuel cells. The single straight channel modified as a complex
**TABLE 3**: Studies that investigated interfacial phenomena in GCs and GDLs of PEMFCs using VOF

<table>
<thead>
<tr>
<th>Reference</th>
<th>Dimension</th>
<th>Component details</th>
<th>Research subject</th>
<th>Related interfacial phenomena</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bao et al. (2014)</td>
<td>3D</td>
<td>A 60 mm-long microchannel with square cross-section of 1 mm × 1 mm</td>
<td>Water initially introduced from the bottom pores of channel</td>
<td>The movement of droplet</td>
</tr>
<tr>
<td>Bazylak et al. (2008a)</td>
<td>2D</td>
<td>A 375 µm × 100 µm gas channel connected to a 25 µm × 200 µm horizontal channel by two channels (25 µm × 100 µm and 50 µm × 100 µm)</td>
<td>Water injected at 0.1 m s⁻¹</td>
<td>Water breakthrough in pores connected to gas channel</td>
</tr>
<tr>
<td>Cai et al. (2006)</td>
<td>3D</td>
<td>A 20 mm-long straight channel with a cross-section of 1 mm × 1 mm with a top surface representing MEA</td>
<td>A single droplet or water film initially placed to the MEA surface</td>
<td>The motion of water droplet or water film on the MEA surface or channel surface</td>
</tr>
<tr>
<td>Cai et al. (2012)</td>
<td>3D</td>
<td>A U-shape channel with round or sharp corner having a length of 4 mm and cross-section of 1 mm × 1 mm channel, 1 mm-wide rib, and water inlet pores with 0.2 mm diameter on the bottom surface</td>
<td>Liquid water injected from inlet pores at 1 m s⁻¹</td>
<td>The evolution of water droplet emergence from the pores</td>
</tr>
<tr>
<td>Carton et al. (2012)</td>
<td>3D</td>
<td>Double serpentine channels with a cross-section of 1 mm × 1 mm straight portion</td>
<td>Droplets placed in the channels</td>
<td>The movement of droplets in the channel</td>
</tr>
<tr>
<td>Chen et al. (2012b)</td>
<td>3D</td>
<td>A 2400 µm-long straight channel with cross-section of 340 µm × 280 µm connecting to a two-layer GDL with a 60 µm × 60 µm × 20 µm water injection pore</td>
<td>Liquid water emerged from the injection pore</td>
<td>The evolution of water droplets injected from the pore</td>
</tr>
<tr>
<td>Chen et al. (2012c)</td>
<td>3D</td>
<td>A straight channel with dimensions of 1000 µm × 300 µm × 300 µm</td>
<td>Liquid water emerged from a series of pores on the GDL surface at a velocity of 1 m s⁻¹</td>
<td>Liquid water distribution</td>
</tr>
<tr>
<td>Chen et al. (2013)</td>
<td>3D</td>
<td>A 340 µm wide, 300 µm-high, and 1200 µm-long rectangle channel with different GDLs</td>
<td>Liquid water injected from a pore at 0.1 m s⁻¹</td>
<td>Droplet behavior</td>
</tr>
<tr>
<td>Reference</td>
<td>Dimension</td>
<td>Component details</td>
<td>Research subject</td>
<td>Related interfacial phenomena</td>
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<tr>
<td>Ding et al. (2013a)</td>
<td>3D</td>
<td>A straight single channel with dimensions of $1 \text{ mm} \times 1 \text{ mm} \times 100 \text{ mm}$ having 20 pores with equal diameter of $250 \ \mu m$ on the bottom surface representing GDL</td>
<td>Liquid water generated from a series of pores at the GDL surface</td>
<td>Two-phase flow patterns</td>
</tr>
<tr>
<td>Ding et al. (2010)</td>
<td>3D</td>
<td>A $1250 \ \mu m$-long straight channel with cross-section of $250 \ \mu m \times 250 \ \mu m$ opening 16 pores with diameter of 50 $\mu m$ representing the GDL microstructure</td>
<td>Liquid water injected from the pores on GDL surface</td>
<td>The evolution of water droplets</td>
</tr>
<tr>
<td>Ding et al. (2011)</td>
<td>3D</td>
<td>A 100 mm-long straight channel with cross-section of $1 \text{ mm} \times 1 \text{ mm}$ opening 320 pores with diameter of 400 $\mu m$ representing the GDL microstructure</td>
<td>Liquid water injected from pores on the GDL surface at velocity of $10^{-4} \text{ m s}^{-1}$</td>
<td>Two-phase flow under different conditions</td>
</tr>
<tr>
<td>Ding et al. (2013b)</td>
<td>3D</td>
<td>Parallel communicating channels with length of 100 mm and cross-section of $1 \text{ mm} \times 1 \text{ mm}$</td>
<td>Liquid water injected from two pores on the GDL surface</td>
<td>Water interface movement under different widths between the two parallel channels</td>
</tr>
<tr>
<td>Ding et al. (2014)</td>
<td>3D</td>
<td>Two parallel channels with length of 50 mm and cross-section of $1 \text{ mm} \times 1 \text{ mm}$ having 10 pores with diameter of 250 $\mu m$ representing pores on the GDL surface</td>
<td>Water injected from the pores</td>
<td>Water distribution</td>
</tr>
<tr>
<td>Dupont et al. (2011)</td>
<td>3D</td>
<td>A rectangle channel</td>
<td>Droplet(s) initially located in the channel</td>
<td>Water droplet movement and coalescence</td>
</tr>
<tr>
<td>Fang et al. (2008)</td>
<td>3D</td>
<td>A 5 mm-long microchannel with cross-section of $500 \ \mu m \times 45 \ \mu m$</td>
<td>Water injected at the bottom of the microchannel with certain velocity</td>
<td>The movement of slug flow</td>
</tr>
<tr>
<td>Fontana et al. (2013)</td>
<td>2D</td>
<td>A 0.05 m-long tapered channel with an inlet height of 0.001 m and an inclination of 0.75$^\circ$ having a series of upper water injection pores with a diameter of 50 $\mu m$</td>
<td>Liquid water injected from several inlets at 0.0126 m s$^{-1}$</td>
<td>The evolution of a series of droplets</td>
</tr>
<tr>
<td>Golpaygan and Ashgriz (2005)</td>
<td>3D</td>
<td>A straight channel</td>
<td>A droplet initially placed in the channel</td>
<td>Droplet deformation</td>
</tr>
</tbody>
</table>
### TABLE 3: Continued

<table>
<thead>
<tr>
<th>Reference</th>
<th>Dimension</th>
<th>Component details</th>
<th>Research subject</th>
<th>Related interfacial phenomena</th>
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<tbody>
<tr>
<td>Golpaygan et al. (2011)</td>
<td>3D</td>
<td>A straight channel initially attached to the bottom surface of channel</td>
<td>A single droplet</td>
<td>Droplet deformation</td>
</tr>
<tr>
<td>He et al. (2010a)</td>
<td>2D</td>
<td>A 1.05 mm × 1 mm straight channel with roughness elements</td>
<td>A liquid water film initially attached to the smooth surface of channel</td>
<td>Liquid water distribution in the channel</td>
</tr>
<tr>
<td>Hossain et al. (2013)</td>
<td>3D</td>
<td>A straight channel with length of 100 mm, width of 1 mm, and height of 1 mm</td>
<td>Water injected at a velocity of 0.0625 m s⁻¹</td>
<td>The evolution of water flow patterns</td>
</tr>
<tr>
<td>Jiao et al. (2006a)</td>
<td>3D</td>
<td>Manifolds with length of 12 mm and cross-section of 2 mm × 2 mm connected by six serpentine channels with straight section length of 10 mm and cross-section of 1 mm × 1 mm</td>
<td>Droplets initially placed at the inlet and water films attached to the channel wall</td>
<td>The movement of water droplets or water films initially placed in the channels</td>
</tr>
<tr>
<td>Jiao et al. (2006b)</td>
<td>3D</td>
<td>Manifolds with length of 20 mm and cross-section of 5 mm × 5 mm connected by five parallel flow fields with straight channel length of 10 mm and cross-section of 1 mm × 1 mm</td>
<td>Droplets initially placed at the inlet and water films attached to the channel wall</td>
<td>The movement of water droplets or water films initially placed in the channels</td>
</tr>
<tr>
<td>Jiao and Zhou (2007)</td>
<td>3D</td>
<td>A unit serpentine channel with a straight section length of 15 mm and a cross-section of 1 mm × 1 mm having 0.1 mm × 0.1 mm × 0.1 mm cubic paths or 0.1 mm-high trapezoid paths with a minimum area of 0.1 mm × 0.1 mm facing the channel or catalyst layer</td>
<td>A liquid water film initially located on the membrane</td>
<td>The evolution of water film initially placed on the membranes</td>
</tr>
<tr>
<td>Jiao and Zhou et al. (2008a)</td>
<td>3D</td>
<td>A unit serpentine channel with a straight section length of 15 mm and a cross-section of 1 mm × 1 mm having 0.1 mm-high trapezoid paths with a minimum area of 0.1 mm × 0.1 mm facing the channel</td>
<td>Liquid water film initially positioned on the catalyst layer</td>
<td>Liquid distribution</td>
</tr>
<tr>
<td>Jiao and Zhou (2008b)</td>
<td>3D</td>
<td>A unit serpentine channel with a straight section length of 15 mm and a cross-section of 0.9 mm × 1 mm having 0.2 mm × 0.2 mm × 0.1 mm cubic paths representing the porous holes on the GDL</td>
<td>A liquid water film initially located on the membrane</td>
<td>The evolution of water film initially placed on the membranes</td>
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</table>

*Interfacial Phenomena and Heat Transfer*
<table>
<thead>
<tr>
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<th>Dimension</th>
<th>Component details</th>
<th>Research subject</th>
<th>Related interfacial phenomena</th>
</tr>
</thead>
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<td>Kang et al. (2011)</td>
<td>3D</td>
<td>A interdigitated flow field with channels of 20 mm length, 2 mm width, and 1.7 mm depth</td>
<td>Liquid water at a flow rate of $1.7 \times 10^{-4}$ was applied at the inlet</td>
<td>Time evolution of liquid water distribution</td>
</tr>
<tr>
<td>Kim et al. (2010)</td>
<td>3D</td>
<td>A 1 mm or 2 mm-wide, 1 mm-high parallel-serpentine channel with sharp or round corner</td>
<td>Two water droplets initially positioned at the rectangular area</td>
<td>The motion of two liquid droplets initially placed in the channel</td>
</tr>
<tr>
<td>Kim et al. (2014)</td>
<td>3D</td>
<td>A 4 mm-long straight channel with rectangle cross-section of $1 \times 0.25$ mm placing two rectangle pores of $50 \times 50 \mu m$</td>
<td>Liquid droplets emerged from the pores</td>
<td>The movement of liquid water interface</td>
</tr>
<tr>
<td>Le and Zhou (2008)</td>
<td>3D</td>
<td>A serpentine channel with 115 mm total path length, 1 mm width, and 1 mm depth</td>
<td>15 spherical droplets initially located in the channel with a radius of 0.4 mm</td>
<td>The motion and deformation of water droplets</td>
</tr>
<tr>
<td>Le and Zhou (2009a)</td>
<td>3D</td>
<td>Interdigitated channels with rectangle cross-section of $1 \times 1$ mm</td>
<td>Spherical droplets initially placed into the channel</td>
<td>The motion process water droplets in spherical shape</td>
</tr>
<tr>
<td>Le and Zhou (2009b)</td>
<td>3D</td>
<td>Serpentine-parallel channels with a total length of 115 mm and a cross-section of $1 \times 1$ mm for each channel</td>
<td>Several droplets initially placed into the channel</td>
<td>Droplet movement, including deformation, coalescence, and detachment</td>
</tr>
<tr>
<td>Le and Zhou (2010)</td>
<td>3D</td>
<td>A stack with parallel channels having rectangle cross-section of $1 \times 1$ mm</td>
<td>12 droplets at single cell channels</td>
<td>Several liquid droplets transported in the stack</td>
</tr>
<tr>
<td>Mancusi et al. (2014)</td>
<td>2D</td>
<td>A 0.05 m-long tapered channel with an inlet height of 0.001 m and an inclination of 0.75° having a series of upper water injection pores with a diameter of 50 µm</td>
<td>Droplets appeared at the beginning with continuous feeding rate</td>
<td>The evolution of a series of droplets</td>
</tr>
<tr>
<td>Minor et al. (2008)</td>
<td>3D</td>
<td>A 1000 µm-long microchannel with cross-section of $250 \times 250$ µm having a 50 µm diameter pore on the GDL surface</td>
<td>Water entered from the pore at velocity of 1 m s$^{-1}$</td>
<td>The evolution of droplet emergence from the pore</td>
</tr>
<tr>
<td>Mondal et al. (2011)</td>
<td>3D</td>
<td>A straight channel with dimensions of $8 \times 1$ mm × $1$ mm</td>
<td>A single droplet initially attached to the bottom surface of channel</td>
<td>The movement of droplet in the channel</td>
</tr>
<tr>
<td>Qin et al. (2012)</td>
<td>3D</td>
<td>A 1 mm-long channel with rectangle cross-section of $0.5 \times 0.2$ mm with three pores at the bottom wall for injection of liquid water</td>
<td>Liquid water provided from the pores connecting to a water reservoir</td>
<td>The movement of water droplet interface</td>
</tr>
<tr>
<td>Qin et al. (2013a)</td>
<td>3D</td>
<td>A 50 mm-long straight channel with a cross-section of $1 \times 1$ mm having an inserted cylindrical needle with a length of 0.7 mm and a diameter of 0.1 mm</td>
<td>A water droplet initially introduced in the channel</td>
<td>Water droplet initially placed on the MEA surface transports through the needle with different dimensions</td>
</tr>
<tr>
<td>Reference</td>
<td>Dimension</td>
<td>Component details</td>
<td>Research subject</td>
<td>Related interfacial phenomena</td>
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<tr>
<td>Qin et al. (2013b)</td>
<td>3D</td>
<td>A 50 mm-long straight channel with a cross-section of 1 mm × 1 mm having an inserted cylindrical needle with a length of 0.7 mm and a diameter of 0.1 mm</td>
<td>A water droplet initially introduced in the channel</td>
<td>Water droplet transport through the needle in the channel</td>
</tr>
<tr>
<td>Qin et al. (2014)</td>
<td>3D</td>
<td>A 50 mm-long straight channel with a cross-section of 1 mm × 1 mm having an inserted hydrophilic plate with a height of 0.7 mm and a length of 1 mm</td>
<td>A water droplet initially introduced in the channel</td>
<td>Liquid water droplet removal from the channel top surface representing MEA surface</td>
</tr>
<tr>
<td>Quan et al. (2005)</td>
<td>3D</td>
<td>A U-shape channel with 20 mm-long straight channel and cross-section of 1 mm × 1 mm film for</td>
<td>Water initially distributed in the channel including droplet, droplets and water different cases</td>
<td>The motion of a single water droplet and water film</td>
</tr>
<tr>
<td>Quan and Lai (2007)</td>
<td>3D</td>
<td>A U-shape channel with sharp corner and dimensions of 1 mm × 0.5 mm × 23 mm attached to a GDL</td>
<td>Constant liquid water was applied on the bottom surface of GDL</td>
<td>Liquid water distribution in the channel</td>
</tr>
<tr>
<td>Quan and Lai (2010)</td>
<td>3D</td>
<td>A portion of interdigitated channel with dimensions of 0.5 mm × 0.5 mm × 12 mm attached to a GDL</td>
<td>Constant liquid water was applied on the bottom surface of GDL</td>
<td>Liquid water distribution in the channel</td>
</tr>
<tr>
<td>Raman et al. (2011)</td>
<td>3D</td>
<td>A 8 mm-long straight channel with cross-section of 1 mm × 1 mm</td>
<td>Single droplet was initially placed in the channel</td>
<td>The movement of droplet in the channel</td>
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<tr>
<td>Shirani and Masoomi (2008)</td>
<td>2D</td>
<td>A straight channel</td>
<td>Droplet initially attached at the channel</td>
<td>The deformation of the droplet interface</td>
</tr>
<tr>
<td>Song et al. (2014)</td>
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<td>A part of serpentine channel with a 3.1 mm-long sharp corner and a cross-section of 1.1 mm × 0.6 mm</td>
<td>Water droplet emerged from pores at the inlet of channel</td>
<td>Time evolution of liquid water interface</td>
</tr>
<tr>
<td>Theodorakakos et al. (2006)</td>
<td>3D</td>
<td>A part of channel</td>
<td>Single droplet initially located in the channel</td>
<td>Water droplet detachment from the pore</td>
</tr>
<tr>
<td>Wang and Zhou (2011)</td>
<td>3D</td>
<td>A parallel flow field with channels of 20 mm length, 2 mm width, 1.7 mm depth</td>
<td>Liquid water at a flow rate of 1.7 × 10⁻⁴ was applied at the inlet</td>
<td>Liquid water distribution during the draining process</td>
</tr>
<tr>
<td>Zhan et al. (2006)</td>
<td>3D</td>
<td>Straight and serpentine channels with length × width × height equal to 11.5 mm × 1 mm × 1 mm and 23 mm × 1 mm × 100 mm, respectively</td>
<td>Single droplet and water film initially in the channels</td>
<td>The transport of a single liquid droplet and water film in channels</td>
</tr>
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</table>
TABLE 3: Continued

<table>
<thead>
<tr>
<th>Reference</th>
<th>Dimension</th>
<th>Component details</th>
<th>Research subject</th>
<th>Related interfacial phenomena</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zhu et al. (2007)</td>
<td>2D</td>
<td>A 1000 μm-long and 250 μm-high microchannel with a 50 μm-wide water injection pore</td>
<td>Water injected at 1 m s(^{-1}) from the pore</td>
<td>The evolution of water droplet emerged from the pore</td>
</tr>
<tr>
<td>Zhu et al. (2008a)</td>
<td>3D</td>
<td>A 1000 μm-long microchannel with cross-section of 250 μm × 250 μm having a 50 μm diameter pore on the GDL surface</td>
<td>Water entered from the pore at velocity of 1 m s(^{-1})</td>
<td>The evolution of water droplet under different conditions</td>
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<td>Zhu et al. (2008b)</td>
<td>2D</td>
<td>A 1000 μm-long and 250 μm-high microchannel with a 0 μm-wide water injection pore</td>
<td>Water injected at a speed of 1 m s(^{-1})</td>
<td>The motion of a water droplet emergence from the injection pore</td>
</tr>
<tr>
<td>Zhu et al. (2010)</td>
<td>3D</td>
<td>A 1000 μm-long microchannel with cross-section of 250 μm × 250 μm having a 50 μm diameter pore on the GDL surface</td>
<td>Water appeared from the pore</td>
<td>The evolution of water droplet with different geometrics</td>
</tr>
<tr>
<td>Zhu et al. (2011)</td>
<td>3D</td>
<td>A 1000 μm-long microchannel with cross-section of 250 μm × 250 μm having a 50 μm diameter pore on the GDL surface</td>
<td>Water was injected from the pore at a velocity of 1 m s(^{-1})</td>
<td>Time evolution of liquid droplet interface</td>
</tr>
<tr>
<td>Ahmad et al. (2013)</td>
<td>2D</td>
<td>GDL</td>
<td>Water was supplied from the inlets of GDL with a velocity of 10 mm s(^{-1})</td>
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</tr>
<tr>
<td>Park et al. (2010)</td>
<td>3D</td>
<td>Reconstructed GDL</td>
<td>The GDL was flooded by stagnant liquid water</td>
<td>Unsteady liquid water behavior</td>
</tr>
<tr>
<td>Suresh and Jayanti (2010)</td>
<td>2D</td>
<td>GDL</td>
<td>Liquid water injected at 0.01 m s(^{-1})</td>
<td>Water transport in ideal GDL</td>
</tr>
<tr>
<td>Yin et al. (2014)</td>
<td>3D</td>
<td>Reconstructed GDL filled in the buffer zone</td>
<td>Liquid water was</td>
<td>Liquid water transport process in the GDL</td>
</tr>
</tbody>
</table>

Compared with single droplet emergence from a pore to simulate liquid water transport from the GDL to the GC, using many droplets is apparently more practical for actual fuel cell operation. Similar to a single droplet, droplets are initially placed in the GC or injected from pores located on the channel wall. The behavior of the two droplets and their inner interaction were investigated by developing VOF models (Kim et al., 2010; Carton et al. 2012; Kim et al., 2014). A simple straight or unit serpentine channel with a round or sharp corner was used. By contrast, Jiao et al. (2006a, 2006b) employed stack channels, which are more complex than straight and unit serpentine channels. The behavior of droplets suspended in the inlet of the stack was analyzed. Le and Zhou (2008, 2009a, 2009b, 2010) applied entire flow fields, including serpentine, interdigitated, serpentine-parallel, and parallel stack channels, with droplets suspended in the channels. The movements at the droplet interfaces were presented. The droplets showed quite diverse behavior in different channels, which indicated the important effect of channel geometry on water management. However, for the suspended droplets, the importance of the GDL from where droplets emerged was ignored. GDL has been proven to considerably influence motion at the interface of the liquid water droplet (Ding et al., 2010, 2011). To simulate the emergence of liquid droplets from the GDL, pores were placed at the surface of the GDL attached to the GC wall. Large pores are preferred in the GDL, as shown by Bazylak et al. (2008a). The arrangement, size, and distribution of pores significantly affect movement at the droplet interface (Ding et al., 2010; Hossain et al., 2013). Ding et al. (2010,
Liu et al. (2011) identified three stages, namely, emergence, accumulation, and detachment, which are common phenomena at the beginning of simulation. Slug and film may appear with prolonged simulation (Fontana et al., 2013; Mancusi et al., 2014). In a subsequent study, Ding et al. (2013a) investigated two-phase flow patterns in a cathode channel in which 20 pores were randomly located at the bottom surface of the channel to represent the water emerging from the pores on the GDL surface. The channel was 10 mm long, which was much shorter than a typical fuel cell channel, so the authors had to amplify the water generation rate. The effects of two-phase flow maldistribution caused by the movement of the droplet interface have also been investigated (Ding et al., 2014). Simple channels, such as straight or serpentine channels, were applied in these studies using pores to mimic the GDL porous structure, and this process limited the information on the movement of the droplet interface in the GC of fuel cells. The channel itself greatly affects the droplet behavior in the GC. For example, Cai et al. (2012) compared the movement of the liquid droplet interface in serpentine channels with different wettability walls. The contact angle altered the water content in the GC and on the wall surface. Song et al. (2014) also investigated the effect of wettability of the channel wall on the movement of the droplet interface. For water removal, a hybrid wall is superior to the hydrophobic case, which is more efficient than the hydrophilic case. Ding et al. (2013b) proposed a communication parallel channel for mitigating flow maldistribution in the GC. Given the GDL, the entire fuel cell channel structure is difficult to implement in the simulation. Thus, either a complex channel with liquid water droplets suspended in the channel or a simple channel with pores on the wall may be used for emerging liquid water. The optimal choice is a combination of these cases, i.e., a complex channel with pores on the wall presenting GDL for emerging liquid water.

Given that liquid water continuously emerges from the GDL, a water film may exist in the GC, especially at large current density. The water film behavior was investigated by initially placing a water film in the computation domain. Quan et al. (2005) analyzed the liquid water distribution by initially attaching a water film to an imaginary MEA and interior surface of a U-shaped channel. They identified the formation of void space. Similar to initially placing a water film in a channel, liquid water continuously injected on the surface of the GDL attached to the GC, which has been adopted to investigate the water behavior in serpentine (Quan and Lai, 2007) and interdigitated (Quan and Lai, 2010) channels, can also achieve a water film. Zhan et al. (2006) presented the motion of a water film initially placed in straight and serpentine channels. Instead of simply presenting the evolution of a water film in the GC, Cai et al. (2006) evaluated the effect of channel wall wettability. Results showed that a hydrophobic surface removes water faster than a hydrophilic one. The latter has stronger surface adhesion, which impedes water removal. Changing the surface property is an effective approach for rapid water removal. Considering the channel surface contact angle, He et al. (2010a) studied the effect of channel surface roughness. Roughness in hydrophilic cases is more efficient for water removal than in hydrophobic conditions. Jiao and Zhou (2007, 2008a) paid more attention on the effects of GDL, including GDL surface wettability and structure. Liquid water transport across the GDL to GC was also investigated by Jiao and Zhou (2008b). They found that the water film can exist on the CL and be destroyed at the turn of the U-shaped channel. The droplets were difficult to remove from the GDL surface because of the combined action of surface and wall adhesions. In their previous studies, Jiao et al. (2006a, 2006b) even applied complex stack channels rather than a straight or unit serpentine channel. Cases with different initial water film distributions were conducted. The proposed channels may provide guidance for the channel design of fuel cells.

### 2.3.4 LB for Channels

As previously introduced, the LB approach is a promising tool for investigating liquid water transport in the GDL of PEMFCs. Thus, this approach can also be a powerful tool for detecting liquid water transport in the GC of PEMFCs. A good example is the pioneering study of Hao and Cheng (2009b), in which a droplet dynamic was conducted in a microchannel. Water droplet formation and the removal process were presented. Similar results were achieved in various VOF simulations (Shirani and Masoomi, 2008; Zhu et al., 2008a, 2010). The diameter of the detached droplet decreases with increasing capillary number. This phenomenon was confirmed in their subsequent work (Hao and Cheng, 2010b) and by the work of Amara and Nasrallah (2015). The deformation of a droplet adhered to a microchannel wall was examined by Hao and Cheng (2010b), as well as by Amara and Nasrallah (2015). Results showed that increasing capillary number leads to strong droplet deformation, which is advantageous for water removal. Salah et al. (2012a, 2012b) used channel design to investigate droplet behavior. A rectangular channel is superior to a
trapezoidal or triangular channel, and a hydrophilic wall is superior to a hydrophobic one. Han and Meng (2012) used serpentine GCs with either a round or sharp turn. The channel with a round turning corner was revealed to be beneficial for liquid water removal, which was consistent with the results achieved in VOF works (Kim et al., 2010; Cai et al., 2012). The interaction of liquid water droplets emerging from two pores in a straight channel (1000 µm × 400 µm) was investigated by Han et al. (2012a). In actual operating fuel cells, obvious two-phase flow occurs in the GC and can be visually observed. In the aforementioned LB models, droplet behavior in GCs is given importance. Given the intrinsic feature of the mesoscopic LB approach, the applied GCs concentrated on the microscopic scale, which should be extended to large-scale channels. Large-scale channels or flow fields can provide a more comprehensive view and deep insight into the water transport.

2.4 Basic Equations in Models

The above sections describe interfacial phenomena in PEMFCs based on observation and modeling. As pointed out by Weber et al. (2014), to study the PEMFC behavior with complex physics at a continuum scale, the governing equations for mass, momentum, energy, and charge transport are needed to be used in the domains or components. Therefore, the basic equations in the models involved interfacial phenomena are presented and discussed in this section. Governing equations are essential parts for continuum and mesoscopic models. The equations in continuum models are used to describe the mass, momentum, energy, and charge transport in PEMFCs. To better understand how the phase interface is considered in the models, related governing equations are also presented.

Continuity equation:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_m
\]  
where \( \rho \) is the density, \( \mathbf{u} \) is the velocity, and \( S_m \) is the source term. The mixture density \( \rho \) can be determined by
\[
\rho = \alpha_l \rho_l + \alpha_g \rho_g
\]
where \( \alpha \) is the volume fraction of each phase (\( l \) represents liquid phase and \( g \) represents the gas phase).

Momentum equation:
\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot [\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho \mathbf{g} + \mathbf{F}
\]
where \( p \) is the static pressure, \( \mathbf{g} \) is gravitational acceleration, and \( \mu \) is the mixture viscosity, which is determined by
\[
\mu = \alpha_l \mu_l + \alpha_g \mu_g
\]
In most VOF models, continuum surface force is used and is given by
\[
\mathbf{F} = \frac{\sigma \alpha_i^2 \mathbf{n} \nabla \alpha_i}{\rho_l + \rho_g}
\]
where \( \sigma \) is the surface tension between phases, and \( k \) is the curvature defined in terms of the divergence of the unit normal of the phase interface \( \mathbf{n} \):
\[
\kappa = \nabla \cdot \mathbf{n} = \nabla \cdot \frac{n}{|n|}
\]
\( n \) corresponds to the surface normal, which can be written as the gradient of volume fraction of phase \( i \):
\[
n = \nabla \alpha_i
\]
In the VOF models, the following volume fraction continuity equation is solved to capture the phase interface:
\[
\frac{\partial \alpha_i \rho_i}{\partial t} + \mathbf{u} \cdot \nabla (\alpha_i \rho_i) = S_{\alpha_i}
\]
where \( \alpha_i \) is the volume fraction of phase \( i \), \( \rho_i \) is the density of phase \( i \), and \( S_{\alpha_i} \) is the source term of phase \( i \).
In LS models, the surface tension is described as
\[
\vec{F} = \nabla \cdot \{ \sigma \left[ I - (\vec{n}_l \vec{n}_l^T) \right] \delta \}
\]
(9)
where \(\sigma\) is the surface tension coefficient, \(I\) is the density matrix, \(\vec{n}_l\) is the interface normal, and the \(\delta\) function is calculated by
\[
\delta = 6|\nabla \phi| |\phi(1 - \phi)|
\]
(10)
\(\phi\) is the LS function that varies between 0 and 1. The tracking of interface between two phases is accomplished by the LS function \(\phi\). The transport of the gas–liquid interface is expressed by
\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \vec{v}) + \gamma \left\{ \nabla \cdot \left[ \phi(1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right] \right\} - \varepsilon \nabla \cdot \nabla \phi = 0
\]
(11)
where \(\gamma\) and \(\varepsilon\) are reinitialization parameters.

The above-mentioned equations are used in continuum models such as the VOF and LS models. The following introduced equations are mainly used in LB or PN models.

Several LB models have been applied to investigate the water transport in PEMFCs, such as Shan and Chen (1993) (SC model) and free energy model of Swift et al. (1995). Using the SC LB model, the fluid flow is described by the evolution of the particle distribution function \(f(r, t)\) in direction \(a\) as follows:
\[
f_a(r + e_a \delta t, t + \delta t) - f_a(r, t) = -\frac{1}{\tau} \left[ f_a(r, t) - f_{eq}^a(r, t) \right] + \delta t F_a(r, t)
\]
(12)
where \(r\) is the position vector, \(t\) is the time, \(\tau\) is the independent relaxation parameter, \(\delta t\) is the time step, \(e_a\) is the discrete velocity, \(f_{eq}^a\) is the equilibrium particle distribution function, and \(F_a\) is the external force. The lattice velocity vector varies in different models such as D2Q9 (two-dimension and 9 discrete velocities) in Zhou and Wu (2010) and D3Q19 (three-dimension and 19 discrete velocities) in Hao and Cheng (2010a).

The equation of state of a nonideal fluid controls the separation of two phases such as liquid and gas phases in PEMFCs. The equation of state is an equation to determine the pressure \(P\), which represents various forms in literature, e.g., the following forms in the model of Chen et al. (2012a):
\[
P = \rho c_s^2 + \frac{3}{2} \sum G_{ii} \psi_i \psi_{ri}
\]
(13)
where \(c_s\) is the sound speed, \(G\) is to control the strength of interaction between phases, and \(\psi\) is the effective density for phase \(i\).

Applying free energy LB models, another distribution function \(g(r, t)\) is required to describe the fluid flow, which can be express as
\[
g_a(r + e_a \delta t, t + \delta t) - g_a(r, t) = -\frac{1}{\tau_g} \left[ g_a(r, t) - g_{eq}^a(r, t) \right]
\]
(14)
where \(\tau_g\) is also an independent relaxation parameter.

To distinguish two phases, the phase parameter \(\varphi\) is solved and given by:
\[
\varphi = \sum_{a=0}^{N} g_a
\]
(15)
where \(N\) is a number that depends on the discrete velocity, e.g., \(N\) equals 9 in the model of Tabe et al. (2009), applying D2Q9.

In the PN models, the water transport is controlled by the capillary pressure, which can be written as
\[
P = -\frac{2\sigma \cos \theta}{r}
\]
(16)
where $\sigma$ is the surface tension, $\theta$ is the contact angle, and $r$ is the mean radius of curvature for the gas–liquid interface. This equation describes the transport of the phase interface.

The governing equations are quite different in the continuum and mesoscopic models. Continuum models have been broadly used for PEMFCs, which cannot handle specific issues. While mesoscopic models have been applied to porous layers in PEMFCs at the pore level, the input of important properties such as permeability and thermal conductivity in mesoscopic models are more difficult than in continuum models. To use the respective advantages such as the complicated physics of continuum models and pore level water transport of mesoscopic models, there is a need for coupling continuum and mesoscopic models. Zenyuk et al. (2015) combined continuum and PN models for better performance predictions. They tried three coupling methods with different cell structures and variables. The three methods were compared and analyzed, and each of these methods had advantages and disadvantages. This is a preliminary attempt, which could be a new trend on modeling of interfacial phenomena in PEMFCs.

2.5 Gas Diffusivity

Gas diffusivity plays an important role with regard to the mass-transport limitations and therefore on the interfacial phenomena. In the GC, the mass transport relies on the convection caused by the supply of reactants. As the reactants are transported to the porous layers, diffusion becomes the main transport pattern. Binary gas diffusivity and effective gas diffusivity significantly affect the mass transport in GC and porous layers, respectively. However, the measurement of gas diffusivity for hydrogen and oxygen is rather difficult to conduct in an operating PEMFC. Therefore, *ex situ* experimental measurements of the effective gas diffusion coefficient have been presented, such as by using a Loschmidt cell (Chan et al., 2012; Shen et al., 2011; Unsworth et al., 2013; Zamel et al., 2010) and electrochemical diffusimetry (Flückiger et al., 2008; Kramer et al., 2008). Baker et al. (2006) used limiting current density for estimation of the gas diffusion coefficient. Yu and Carter (2010) applied a simplified apparatus to measure the oxygen diffusivity in PEMFC electrodes. In addition to measurements based on experiments, there has been a number of work based on modeling, such as the PN model (Wu et al., 2010c), the analytical model (Shou et al., 2013), and correlation (Zamel et al., 2009). Shi et al. (2010a, 2010b) estimated binary oxygen diffusivity and effective hydrogen diffusivity of GDLs in PEMFCs by using a fractal model. Although abundant works have been conducted to estimate the effective gas diffusivity, few involve interfacial phenomena. Therefore, the combination of estimation of gas diffusivity regarding mass-transport limitations and interfacial phenomena in PEMFCs is recommended.

3. Heat Transfer in PEMFCs

3.1 Heat Sources and Temperature in PEMFCs

Heat is released during fuel cell operation. Various sources contribute to heat generation, including irreversible electrochemical reaction heat, entropic heat, latent heat of water phase change, and Joule heat. Irreversible heat stems from the irreversibility of electrochemical reactions. Entropic heat is the difference between the chemical energy of reactants and maximum usable work according to the second law of thermodynamics, whereas Joule heat is produced from the electronic and protonic currents corresponding to the resistance of fuel cell components (Ju et al., 2005). Latent heat results from the change in water phase, such as water condensation or ice formation at freezing conditions. Entropic heat accounts for the major portion (up to ~50%) of heat sources (Ju et al., 2005; Jiang et al., 2007). Earlier analysis (Lampinen and Faminan, 1993) showed that the oxygen electrode is heated. A large amount of heat is generated in the CCL because of the exothermal reaction occurring in the layer that creates a peak temperature within the layer. This phenomenon has been verified by numerous thermal models (Djilali and Lu, 2002; Ju et al., 2005; Steinkamp et al., 2008; Falcao et al., 2009; Afshari and Jazayeri, 2010; Zamel and Li, 2010; Xing et al., 2014). This phenomenon is also supported by the temperature distribution illustrated in the models (Matamoros and Bruggemann, 2006; Burheim et al., 2013; Dadda et al., 2013, 2014), in which the maximum temperature is located in the membrane close to the CCL. However, Ramousse et al. (2009) suggested that the oxygen reduction reaction is endothermic. The reversed result may lead to different thermal gradients in fuel cells. The temperature distribution in fuel cells is generally expected to be nonuniform because of heat generation. This nonuniformity is embodied in distributions not only across fuel cells, but also on the in-plane direction of components, e.g., the nonuniform temperature distribution...
on the membrane presented by Dadda et al. (2013, 2014). The temperature increases from the anode to the membrane and then decreases from the membrane to the cathode. The temperature profile is almost linear at the anode and cathode sides, mainly because of heat conduction, and the temperature in the membrane is nonlinear because of Joule heat and the latent heat of water phase change (Rowe and Li, 2001; Djalili and Lu, 2002; Ramoussé et al., 2005). The trend of the temperature distribution in fuel cells may lead to hot spot formation in the membrane. To avoid membrane failure caused by hot spots and obtain better performance, highly uniform temperature distributions are desired.

The generated heat increases the operating temperature of the fuel cell. Higher temperature may improve the performance of a fuel cell. However, excessively high temperature overheats the components of a fuel cell, especially the membrane. The generated heat should be promptly removed to avoid membrane dehydration. By contrast, very low operating temperature is undesirable because low temperature decreases proton conductivity and electrochemical reaction kinetics. Consequently, heat management is an important issue for safe and long-term operation of fuel cells. Understanding heat transfer is essential for improved heat management in PEMFCs. Directly investigating heat transfer inside fuel cells is difficult because of their structure. This characteristic facilitates the development of modeling because heat transfer can be considered by introducing an energy equation. Not all heat resources are considered in most models. These models, such as studies on latent heat of water phase change (Ying et al., 2005a; Wang and Ouyang, 2007; Hottinen and Himanen, 2007; Ismail et al., 2013), have ignored one or more certain heat resources depending on the research subject.

3.2 Effect of Components on Heat Transfer

PEMFCs show diverse heat transfer phenomena, such as heat conduction between components, convective heat transfer between components and fluid flow, and heat release and absorption accompanying the change in water phase. Given that heat is generated by the electrochemical reaction in the CL, heat will be conducted on the two sides of components from the CL because of the temperature gradient. In addition to heat conduction, convective heat transfer caused by fluid flow also exists, especially in the GC. These heat transfer phenomena are related to the fuel cell components. The property of a material used for components plays an important role in heat transfer. For example, the thermal conductivity of the GDL significantly affects heat transfer, thereby leading to different temperature distributions.

The GDL, one of the important components in PEMFCs, remarkably affects heat transfer. Kopanidis et al. (2011) showed that the property of the GDL considerably affects hot spot prediction. Hot spot formation may cause membrane failure. Heat should be effectively removed to prevent hot spot formation. Electrochemical reaction heat, which is the main heat source, is primarily conducted from CL to GC through GDL. The thermal conductivity of the GDL plays a vital role in heat conduction, which may alter features in fuel cells such as temperature and performance. Different temperature distributions in fuel cells (Pharoah and Burheim, 2010) and cell performances (Bapat and Thynell, 2008) for various GDL thermal conductivities have been demonstrated. Wang et al. (2012) also pointed out that performance is significantly affected by the thermal conductivity of the GDL with a low convective heat coefficient. Moreover, the GDL has anisotropic thermal conductivity because of the inherent anisotropic porous carbon fiber (He et al., 2010b). This anisotropic thermal conductivity causes different heat transfer characteristics in diverse directions. The thermal behavior of isotropic GDL differs from that of anisotropic GDL (Pasaogullari et al., 2007; Ju, 2009; Cao et al., 2013). Results predicted by models with anisotropic GDL are more accurate than those by models with isotropic GDL (Pasaogullari et al., 2007; Cao et al., 2013). The through-plane thermal conductivity of an anisotropic GDL differs greatly from the in-plane thermal conductivity. The difference results in different temperature gradients. Generally, the temperature gradient in the through-plane direction is much larger because of the larger conductivity (Sun, 2012). Even for the in-plane thermal conductivity, the direction perpendicular to the channel is more important than that along the channel direction (He et al., 2010b). Bapat and Thynell (2006) developed a 2D model to investigate the effects of anisotropic thermal conductivity. They suggested that high in-plane thermal conductivity is preferable because the temperature distribution in the GDL with a high in-plane thermal conductivity is much more uniform than that in GDL with a low in-plane thermal conductivity. They subsequently extended the model to a two-phase model, and through-plane thermal conductivity was considered (Bapat and Thynell, 2008). The fuel cell showed improved performance with appropriate temperature for a GDL with combined high in-plane and low through-plane thermal...
conductivities. Alhazmi et al. (2013) simply fixed the in-plane (through-plane) thermal conductivity to a certain value and varied the through-plane (in-plane) thermal conductivity to study the effect of anisotropic thermal conductivity. Uniformity of the temperature distribution was enhanced with the increase in in-plane or through-plane thermal conductivity. The anisotropic thermal conductivity influences the heat transfer in PEMFCs, especially the temperature. In future models or numerical simulations that involve heat transfer in fuel cells, an anisotropic thermal conductivity GDL should be considered for more accurate prediction.

GC is also an important component in fuel cells, which distributes fuel and offers passages for water removal. Convection heat transfer and heat conduction simultaneously occur in flow fields. Convection heat transfer occurs in channels because of the fuel flow. Heat conduction exists because heat is transported between components. Thermal conductivity and channel structure are important in heat transfer. Materials with high thermal conductivity are applied to enhance the heat conduction in a flow field. Graphite is widely used for flow fields. For heat transfer in channels, researchers prefer to start from the channel structure or flow field design. Channel width is a sensitive parameter (Pharoah and Burheim, 2010). Moderate channel width is preferred because a very small or big channel open ratio is an obstacle for strong convection heat transfer (Ying et al., 2005b). Fontana et al. (2011) investigated the effects of flow field on heat transfer. The inclination of the flow channel was regarded as a variable parameter. The deeper the channel was, the more oxygen was supplied at the CL, and the more heat was produced. Consequently, the inclination mainly affected the temperature distribution at the cathode side given the different heat productions. Perng and Wu (2009) inserted plates into channels to enhance the heat transfer in these channels. Enhanced heat transfer was obtained with the insertion of a baffle plate. They also tested tapered channels with baffle (Perng and Wu, 2011; Perng et al., 2014), which offered similar benefits. A wavelike channel applied by Kuo and Chen (2006) improved the heat transfer performance, considering that they obtained lower and improved uniform temperature distribution. In a subsequent work, Kuo and Chen (2007) explained that the improved heat transfer may have been caused by an increase in flow interruption, a reduction in thermal boundary layer, and an elevated velocity gradient near the GDL boundary. These factors are deeply affected by the flow field design, e.g., the sub-rib convection velocity distribution near the GDL was altered by applying a new flow field design, which is distinct from the conventional one (Wang et al., 2009, 2010a, 2010b). Therefore, the flow field design can be optimized to enhance heat transfer in fuel cells.

### 3.3 Interaction Between Water and Heat Transfer

Heat transfer is intrinsically coupled with water transport because heat and water are simultaneously produced during an electrochemical reaction. Although abundant heat is removed through heat conduction, a certain amount of heat remains and is absorbed by the generated liquid water. The water becomes water vapor after heat absorption, and the vapor is transported to the GDL. As the vapor transports to the relatively cold GC through the GDL, it condenses into liquid water in the form of droplets because of the GDL structure and release of heat. The thought remains hypothetical because no one has really observed or measured such phase change inside a GDL. A dendritic flow is thought to exist in the GDL (Litster et al., 2006; Medici and Allen, 2009). Fig. 5 shows a schematic of the dendritic flows in GDL. The heat removal mechanism is known as heat pipe effect (Wang and Wang, 2006), which has been confirmed by several studies (Weber and Newman, 2006; Afshari and Jazayeri, 2009; Ju, 2009; Wang and Chen, 2011; Bhaiya et al., 2014). The heat pipe effect is also called a phase-change–induced flow (Khandelwal et al., 2009), which has attracted much research attention (Kim and Mench, 2009a, 2009b; Hatzell et al., 2009). Another heat pipe effect (Meng, 2007a; Pasaogullari et al., 2007; Tabuchi et al., 2010; Khajeh-Hosseini-Dalasm et al., 2010) perhaps exists, which occurs in the flow channels at the in-plane direction. Water absorbs heat and evaporates at a high-temperature GC region. The vapor created by evaporation moves to the colder flow field land or rib area and then condenses into liquid water with heat release. The heat pipe effect is due to the temperature gradient, and it enhances heat transfer because of the latent heat of water condensation. Although all the studies on the heat pipe effect are based on models, they suggest that heat and water interact with each other. Fuller and Newman (1993) suggested that thermal factors must be considered when analyzing water management. He et al. (2009) demonstrated that liquid water hinders heat transfer in CL or GDL. Meanwhile, water phase change has been found to influence the heat and temperature distribution of a cathodic reaction (Afshari et al., 2010; Herrera et al., 2012). Heat transfer coupled with water transport affects the transient response of PEMFCs (Meng, 2007b; Wu et al., 2007; Hwang et al., 2012). Heat transfer evidently interacts with...
water transport. However, this intricate interaction remains unclear. More comprehensive modeling and experiments are warranted for enhanced understanding of the interaction of heat and water transport, such as the hybrid model coupling continuum and PN models proposed by Zenyuk et al. (2015).

3.4 Cooling for PEMFC

Heat should be removed from fuel cells because of the exothermic reaction. Heat exchanges between components and fluids occur in fuel cells (Nguyen and White, 1993; Hwang, 2006; Hwang et al., 2006; Hwang and Chen, 2006; Chao and Hwang, 2006; Min, 2010), and heat is removed by the reactants and products. Heat is also removed to the end plate via heat conduction. The end plate is directly exposed to the ambient environment to induce heat convection. Convection can be used in miniature fuel cells (Litster et al., 2006). A heat exchanger (Yi and Nguyen, 1998) or coolant (Dannenberg et al., 2000) can also be used for heat removal in fuel cells. For most fuel cells, especially air-breathing fuel cells, the convection is sufficiently effective. For high-temperature or large-active-area PEMFCs, the convection becomes insufficient; thus, a cooling system operating on air or water is applied to sufficiently regulate the fuel cell temperature (Yu and Jung, 2008; Jung et al., 2008; Park and Min, 2012; Chippar and Ju, 2012). The internal heat transfer in a single PEMFC has attracted much attention, whereas research on PEMFC stacks mainly focused on cooling issues. A PEMFC stack for industrial, automotive, and other applications requires high power output. Given this context, cooling the PEMFC stack becomes highly important. Various cooling systems, such as air cooling including natural convection (Koh et al., 2005; Huang et al., 2008; Wan Mohamed et al., 2010) and forced convection (Strahl et al., 2011; Akbari et al., 2012; Reddy and Jayanti, 2012), water cooling systems (Pandiyan et al., 2008; Vasu and Tangirala, 2008; Song et al., 2011; Cozzolino et al., 2011; Hwang, 2013), heat spreader (Wen et al., 2011), and phase change material (Sasmito et al., 2013) are applied to PEMFC stacks. Natural convection, as a simple and passive method, may be insufficient for controlling temperature, especially at high current (Koh et al., 2005; Huang et al., 2008). Other cooling methods highly depend on the external thermal management system. Although energy consumption units, such as a fan or coolant pump, in the external thermal management system increase the system energy consumption and complexity, these cooling systems are still applied because of their effective temperature control. Given that the present study focuses on the heat transfer in PEMFCs, cooling of the PEMFC stack is not
introduced in detail. For more details on PEMFC stack cooling, one may prefer to a review study of Zhang and Kandlikar (2012).

4. SUMMARY

Water and heat management is a critical issue for PEMFCs. Abundant strategies have been developed for enhanced water and heat management in PEMFCs in the past decades. Understanding water transport and heat transfer in PEMFCs is important to implement these strategies according to operating conditions and designs. Interfacial phenomena in PEMFCs are closely related to water transport. More specifically, interfacial phenomena involve the water phase interface. In this work, studies related to interfacial phenomena or heat transfer in PEMFCs were reviewed. The main conclusions are drawn as follows:

1. The interfacial phenomena in CL still require further effort. Only a few studies have been conducted on the interfacial phenomena in CL, including experimental and modeling work. Generally, a membrane electrolyte assembly is applied, and the CL is sandwiched by the membrane and GDL in the PEMFC. As a result, the interfacial phenomena in CL are difficult to investigate.

2. Simulation studies on interfacial phenomena are limited to a local position in PEMFCs, such as PN for GDL and LS for GC. In LB and PN, which are preferred for porous GDL application, liquid water transport is analyzed at the pore scale or mesoscopic level. Phase tracking is unnecessary in LB and PN models, considering that the phase interface can be automatically maintained. LS and VOF approaches are mainly applied to investigate liquid water dynamics and transport in GCs. The liquid water phase interface is tracked using a complex method. Models apply simplified components as a computational domain, which has a limited time scale and physical size. Comprehensive models that contain complex interfacial phenomena, electrochemical reaction, long-term calculation, and large physical size should be studied in future investigations on PEMFC water management, such as the hybrid model containing complex interfacial phenomena.

3. In situ or ex situ experimental observations provide visual views of the liquid water droplet or two-phase flow in the components of PEMFCs, which are vital for understanding the water transport mechanism in fuel cells. Although in situ two-phase flow observation provides a comprehensive view in the flow field of PEMFCs, mere observations are insufficient to provide deep insight into the water transport mechanism. Ex situ experiments have been conducted to observe droplets in CCL and GDL and two-phase flow in GC. However, ex situ experiments use simplified equipment without the coupling electrochemical reaction, which restricts the contribution to fuel cell application.

4. The properties of the different components significantly influence heat transfer. Investigations on heat transfer are mostly based on models. Experiments should be performed to accurately determine properties, such as thermal conductivity of components, for optimizing the design of PEMFCs. The determination of accurate properties also guarantees the reliability of numerical simulations, as unknown and invalidated properties are used in simulation models.

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REFERENCES


Hatzell, M. C., Turhan, A., Kim, S., Hussey, D. S., Jacobson, D. L., and Mench, M. M., Quantification of temperature driven flow in...


Meng, H., A two-phase non-isothermal mixed-domain PEM fuel cell model and its application to two-dimensional simulations, *J. Power Sources*. 


Wang, X. D., Duan, Y. Y., Yan, W. M., Lee, D. J., and Su, A., Channel aspect ratio effect for serpentine proton exchange membrane


