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Numerical study of gas purge in polymer electrolyte membrane fuel cell

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ABSTRACT

Gas purge for eliminating water from gas diffusion layer (GDL) and membrane is of great importance for polymer electrolyte membrane fuel cell (PEMFC) start-up at subfreezing temperature. A gas purge model was developed to investigate the water transport phenomenon in GDL and membrane. In simulations, hydrogen and air were used as purge streams in anode and cathode, respectively. Effects of purge conditions on gas purge were numerically studied. In addition to relative humidity, flow rate and temperature, the flow configuration of purge gases was studied for the first time. In order to improve purge performance, several purge protocols were proposed and discussed in detail with respect to purge effectiveness and energy saving.

1. Introduction

Polymer electrolyte membrane fuel cell (PEMFC) is an energy conversion device which can directly convert the chemical energy of fuel into electric power through electrochemical reaction. PEMFC is a promising power source for portable device, transport and distributed generation with advantages of high efficiency, no pollution and low noise [1]. In the past decades, much attention has been posed on the development of fuel cell vehicles. In the regard of fuel cell vehicles, successful and rapid start-up of fuel cell at sub-zero temperature, also called cold start, is of a great importance for their commercialization in automobile [2]. During operation, water is produced in cathode catalyst layer (CL) due to electrochemical reaction. When the membrane is fully hydrated, product water will resident in catalyst layer and formed ice or frost during cold start, which will block the catalyst layer and result in shutdown of fuel cell. If the membrane is rather dry, product water will diffuse into membrane and be stored there. In this case, the cell temperature may succeed to rise above 0 °C before the catalyst layer is totally blocked [3]. Therefore, every time a fuel cell is shut down, it is necessary to remove water in gas diffusion layer (GDL), catalyst layer and membrane by gas purge in order to create enough space for water storage during cold start.

Numerous studies have been reported on the experiments of gas purge. Tajiri et al. [4] developed a reproducible experimental method to characterize the drying process of gas purge by measuring the variation of high-frequency resistance (HFR). Ge and Wang [5] measured the cell high-frequency resistance (HFR) during gas purge with different purge durations, and found that the cell HFR significantly influences the amount of cumulative product water in isothermal cold start. Lee et al. [6]developed a consistent and repeatable experimental method to determine local water content by using micro sensors to measure local HFR, and investigated water transport phenomena during gas purge in fuel cells. Lee et al. [7] developed a method for measuring the amount of residual water in the fuel cell, and use this method as well as HFR measurement to investigate the water removal characteristics. Sinha et al. [8] employed X-ray microtomography to quantify liquid water distribution in the gas diffusion layer and calculated the water removal rate with purge time at room temperature. St-Pierre et al. [9] developed a residence time distribution method and demonstrated its capability for detecting liquid water in gas channel and electrode. Cho and Mench [10] developed a special test system to investigate the fundamental behavior of evaporative water removal from diffusion media (DM) during gas purge with minimal in-plane gradients in saturation temperature. Based on the experimental results, they further developed a generic plot of purge efficiency, and proposed a purge protocol that applied composite flow rates of purge gas to enhance durability and reduce parasitic energy losses. Cho and Mench [11] also studied the effects of material properties, such as polytetrafluoroethylene (PTFE) content and geometric pore structure, on evaporative water removal from diffusion media, and compared the effects of phase-change-induced (PCI) flow and capillary flow on water removal. They also developed new methods to measure internal liquid flow rate and irreducible saturation. With ex situ test methods developed in [10,11] and neutron radiography (NR), Cho and Mench [12]

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Nomenclature

Latin characters

a	water activity [–]
A	area [m^2]
C	concentration [mol m^{-3}]
D	diffusivity [m^2 s^{-1}]
EW	equivalent weight [kg mol^{-1}]
f	volume fraction of water in the membrane [–]
k	mass transfer coefficient [m s^{-1}]
L	length [m]
M	molecule weight [kg mol^{-1}]
n	Bruggemann factor [–]
P	pressure [Pa]
R	resistance or universal gas constant [Ω] or [J K^{-1} mol^{-1}]
s	saturation [–]
S	source term [s^{-1}]
t	time [s]
T	temperature [K]
V	molar volume [m^3 mol^{-1}]
w	width [m]
x	distance away from cathode inlet [m]

Greek characters

δ	depth [m]
ε	porosity or volume fraction [–]
κ	electrical conductivity [S m^{-1}]
λ	water content [–]
ρ	density [kg m^{-3}]
ϕ	relative humidity [–]

Subscripts and superscripts

0	initial value
a	anode
air	air
avg	average value
c	cathode
cell	fuel cell
chan	channel
CL	catalyst layer
d	desorption
dry	dry membrane
eff	effective value
eq	equivalent value
g	purge gas
GDL	gas diffusion layer
H_2	hydrogen
H_2O	water
l	liquid water
land	land
m	ionomer
mem	membrane
o	reference value
sat	saturated water vapor
total	total value
V	volume
w	water
air	relative humidity
ϕ	relative humidity [–]

investigated the coupled effects of land to channel width ratios and diffusion media (DM) structure on the evaporative water removal during gas purge. Tang et al. [13] used in situ neutron imaging to investigate the gas purge performance for different wettability of flow channel, and found that super-hydrophilic coating on the landings and super-hydrophobic coating on the channels helped to improve water removal. Owejan et al. [14] investigated water transport in PEMFC by using ex situ and in situ experiments and proposed a one-dimensional model to calculate the effectiveness of cathode purge for water removal based on the experimental results.

It is also important to study effective purge methods. Kim et al. [15] proposed a new purge method that added a small amount of hydrogen into the dry air. Due to the hydrogen–oxygen catalytic reaction, a large amount of heat was generated, which facilitated water evaporation in CL and GDL. Kim et al. [16] proposed a new and more effective purge method that used a sudden pressure reduction to remove residual water in membrane electrode assembly (MEA) and GDL, and verified the purge performance via several techniques, including cold start experiments and durability tests.

Since numerical simulations can provide information that is difficult to obtain from experiments, much efforts have been devoted to the development of gas purge models. Sinha and Wang [17] proposed an analytical purge model to describe the GDL drying and membrane drying process in the cathode, and provided fundamental insight into gas purge phenomena. The predicted results were verified through tomographic experiments. Based on the analytical model presented by Sinha and Wang [17], Ito et al. [18] developed a modified model to investigate the water removal behavior in GDL and membrane during preswitching gas purge for unitized reversible fuel cells (URFCs). Sinha and Wang [19] developed a more comprehensive three-dimensional two-phase transient gas purge model. The model accounted for capillary transport of liquid water, vapor diffusion, and water transport between anode and cathode through the membrane. Khandelwal et al. [20] developed a transient two-phase computational model to describe water redistribution in PEMFC after shutdown, which for the first time included thermo-osmotic flow in the electrolyte membrane and phase-change induced (PCI) flow in the porous media, and investigated impacts of thermo-osmotic, capillary and PCI flow on water removal. Wang et al. [21] developed a dynamic three-phase transport model to study water uptake and transport process in PEMFC during cold start and shutdown. They ran simulation to analyze the purge time and energy consumption as a function of initial stack temperature and saturation level of GDL for drying the membrane to a target level during shutdown.

In the relevant literature, nitrogen was usually used as purge gas in research on gas purge or cold start, as reported in [4,5,7,11–14,17–19,22–25]. However, an additional gas tank and pipes are required for nitrogen gas purge, which will definitely increase the complexity and the weight of the fuel cell system. As a result, the cost of the fuel cell vehicle may increase whereas the cruising range may decrease. In comparison, gas purge with hydrogen in the anode and air in the cathode is a better choice, because no extra device is required. However, research on gas purge with hydrogen and air is scarce [15,16]. Therefore, the gas purge process using hydrogen and air is investigated in this work.

The purge model presented by Sinha and Wang [17] and Ito et al. [18] considered only cathode purge. In this study, we further developed their model to predict gas purge process for both anode and cathode and water transport through the membrane. To validate our model, numerical predictions of HFR vs purge time are