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Characteristics of PEMFC operating at high current density with low external humidification

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ABSTRACT

A three-dimensional multiphase numerical model for proton exchange membrane fuel cell (PEMFC) is developed to study the fuel cell performance and water transport properties with low external humidification. The results show that the sufficient external humidification is necessary to prevent the polymer electrolyte dehydration at low current density, while at high current density, the water produced in cathode CL is enough to humidify the polymer electrolyte instead of external humidification by flowing back and forth between the anode and cathode across the membrane. Furthermore, a steady anode circulation status without external humidification is demonstrated in this study, of which the detailed internal water transfer path is also illustrated. Additionally, it is also found that the water balance under the counter-flow arrangement is superior to co-flow at low anode external humidification.

1. Introduction

Proton exchange membrane fuel cell (PEMFC) is a device that can directly convert the chemical energy to electric energy. Due to its many advantages such as low emissions, high power density and so on [1,2], it has attracted considerable attention in a wide range of applications. However, the water management in PEMFC is still a vital challenge [3]. The polymer electrolyte must be hydrated enough to effectively facilitate the proton transfer process inside [3,4], otherwise the high ionic resistance will degrade the performance of PEMFC severely. Therefore, to ensure the polymer electrolyte hydration, the inlet reactant gas is usually humidified through the external humidifier, which makes the total fuel cell system heavier, more expensive and complicated [5,6]. Besides this method, internal humidification (or self-humidification) is another effective method, which refers to that the water produced in the cathode catalyst layer (CL) is reasonably retained to humidify the polymer electrolyte [6,7]. And this method can remove the humidifier from the fuel cell system, which is more beneficial to commercialization. Therefore, to remove the external humidifier, the effect of the inlet relative humidity on the performance of PEMFC deserves to be investigated carefully, especially the low inlet relative humidity.

So far, many researches have been implemented to study the performance of PEMFC with different inlet relative humidity. Some experiments and numerical simulations [8–12] have been carried out and it is found that the performance of inlet gas fully humidified in cathode was worse than moderately humidified under a certain condition. Because improving the inlet relative humidity can reduce the inlet reactant gases concentration and increase the mass transfer resistance at higher current density. However, extremely low relative humidity and even no external humidification at cathode inlet would lead to the polymer electrolyte dehydration, so the fuel cell performance would decline [13–16]. Meanwhile, Weng et al. [13] and Jeon et al. [14] found that fuel cell showed fairly uneven performance and temperature distribution along the gas flow direction under low external humidification at cathode inlet. Nevertheless, the experiment result of Jeon et al. [14] showed that extremely high relative humidity at cathode inlet could also lead to the uneven problems due to the liquid water flooding. Takalloo et al. [17] indicated that the external humidification at anode inlet was more necessary than the cathode inlet, because the cathode could produce water and should avoid from flooding. Buchi et al. [18] and Williams et al. [19] successfully operated the PEMFC without external humidification, but at the cost of seriously decreasing the fuel cell performance.

As mentioned before, the effect of inlet gas relative humidity on the performance of PEMFC has been revealed in many researches. And these researches pointed that the fuel cell performance could not be maintained at extremely low external humidification. However, with the development of PEMFC, its current density becomes higher and higher. Operated at high current density, sufficient water will be produced in the cathode CL to effectively humidify the polymer electrolyte in cathode. Meanwhile, the net water flux direction across the membrane might be optimized (back diffusion and electro-osmotic drag)

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Nomenclature

A	area (m^2)
a	water activity
C_i	gas species molar concentration (mol m^{-3})
$C_{H_2}^{ref}$	reference hydrogen concentration (mol m^{-3})
$C_{O_2}^{ref}$	reference oxygen concentration (mol m^{-3})
D_i	gas species diffusivity (m^2 s^{-1})
D_d	dissolved water diffusivity (m^2 s^{-1})
E_{rev}	reversible voltage (V)
EW	equivalent weight of ionomer (kg mol^{-1})
F	Faraday's constant (C mol^{-1})
$Flux$	mass flux (kg m^{-2} s^{-1})
h	latent heat coefficient (J mol^{-1})
H	height (mm)
I^{ref}	reference current density (A m^{-2})
I_{ion}	ionic current density (A m^{-2})
$J_{0,a}^{ref}$	anode reference exchange current density (A m^{-3})
$J_{0,c}^{ref}$	cathode reference exchange current density (A m^{-3})
K	intrinsic permeability (m^2)
k_g	gas phase relative permeability
k_l	liquid phase relative permeability
k^{eff}	effective thermal conductivity (W m^{-1} K^{-1})
L	length (mm)
M	mole mass (kg mol^{-1})
P	pressure (Pa)
P_c	capillary pressure (Pa)
R	universal gas constant (J mol^{-1} K^{-1})
RH	relative humidity
S	source term (kg m^{-3} s^{-1} or mol m^{-3} s^{-1})
ΔS	entropy change (J mol^{-1} K^{-1})
s	liquid water volume fraction
T	temperature (K)
u	velocity (m s^{-1})
	output voltage (V)
W	width (mm)
x	X direction
Y_i	gas species mass fraction
y	Y direction
z	Z direction

Greek letters

α_a	anode transfer coefficient
α_c	cathode transfer coefficient
γ	phase change rate (s^{-1})
δ	thickness (μm)
ε	porosity
η	overpotential (V)
θ	contact angle (°)
κ_e	electric conductivity (S m^{-1})
κ_{ion}	ionic conductivity (S m^{-1})
λ	membrane water content
μ	dynamic viscosity (kg m^{-1} s^{-1})
ξ	stoichiometric ratio
ρ	density (kg m^{-3})
σ	surface tension coefficient (N m^{-1})
φ_e	electric potential (V)
φ_{ion}	ionic potential (V)
ω	ionomer volume fraction

Subscripts and superscripts

0	standard state
a	anode
act	activation
c	cathode
Ch	channel
CL	catalyst layer
d-v	membrane water to vapour
e	electrical
eff	effective
eq	equilibrium state
g	gas phase
GDL	gas diffusion layer
H_2	hydrogen
H_2O	water
i	gas species
in	inlet
ion	ionic
l	liquid water
m	mass
mem	membrane
MPL	micro porous layer
mw	membrane water
O_2	oxygen
p	pressure
ref	reference state
sat	saturation state
T	temperature
v	vapour
v-l	vapour to liquid water

[20–23], which could be employed to humidify the polymer electrolyte in anode. Therefore, the fuel cell performance will present some differences at low external humidification. In this study, the performance and water transport properties of PEMFC under high current density with low external humidification is studied carefully. Furthermore, a steady anode circulation status without external humidification is proposed, and the effects of counter-flow and co-flow on the fuel cell performance and water transport properties are also discussed.

2. Numerical model

2.1. Physical problem

The three-dimensional computational domain in this study includes eleven parts: anode/cathode bipolar plate (BP), anode/cathode flow channel, anode/cathode gas diffusion layer (GDL), anode/cathode micro porous layer (MPL), anode/cathode catalyst layer (CL) and membrane (Fig. 1). Half of a straight-channel single cell is considered to save the computational time with the symmetrical boundary condition utilized. Additionally, the related cell physical parameters and operation conditions are listed in Table 1.

2.2. Conservation equations

There are essential conservation equations developed in this model, to describe the electrochemical electrode kinetics and the two-phase fluids in channel and porous media. All the conservation equations in this model are listed as follows.

Mass of gas mixture (solved in Anode/Cathode Channel, Anode/Cathode GDL, Anode/Cathode MPL, Anode/Cathode CL)

$$\frac{\partial}{\partial t}(\varepsilon(1-s)\rho_g) + \nabla\cdot(\rho_g \vec{u}_g) = S_m \quad (1)$$