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Modeling of hydrogen alkaline membrane fuel cell with interfacial effect and water management optimization

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ABSTRACT

In this study, a whole-cell 3D multiphase non-isothermal model is developed for hydrogen alkaline anion exchange membrane (AAEM) fuel cell, and the interfacial effect on the two-phase transport in porous electrode is also considered in the model. The results show that the insertion of anode MPL, slight anode pressurization and reduction of membrane thickness generally improve the cell performance because the water transport from anode to cathode is enhanced, which favors both the mass transport and membrane hydration. The effect of cathode MPL is generally insignificant because liquid water rarely presents in cathode. It is demonstrated that slight pressurization of anode, which might not lead to apparent damage to the membrane, can effectively solve the anode flooding and cathode dryout issues.

1. Introduction

Alkaline anion exchange membrane (AAEM) fuel cells, with solid electrolyte and alkaline environment suitable for non-precious-metal catalysts, are currently gathering renewed interests and becoming an alternative to other approaches to low temperature fuel cells [1–3].

In the past several years, active researches focused on the improvement of the chemical and mechanical stability and transport properties of AAEMs, to provide fundamental understanding of the anion conducting systems and make these properties compete with proton exchange membranes (PEMs) [4–7]. However, the conductivity of AAEM to date is still lower than its counterpart PEM, because of the lower conductivity of hydroxide in water than proton [6,7]. Moreover, recent experiment observed that in high current density operation, the mass transport limitation of water (water is consumed by reaction and electro-osmotic drag in cathode) rather an oxygen becomes the major performance loss, and the scenario is worse if oxygen is not humidified [8]. As mentioned above, water management of AAEM fuel cell is complicated and critically important because of the requirement of membrane hydration to maintain sufficient hydroxide conductivity, as well as the consumption of water in cathode and the reversed electro-osmotic drag (from cathode to anode).

Different from the active studies in PEM fuel cell water management [9–12], few studies for AAEM fuel cell water management could be found in literature. Weinzierl and Krewer [13] developed a mathematical model to analyze the water management in AAEM direct methanol fuel cell (DMFC), and showed that the requirement of cathode water supply increases with the increment of current density. Steady-state and transient 3D models for hydrogen AAEM fuel cell anode was also developed [14,15], and based on this model, Jiao et al. [16] developed a whole-cell 3D multiphase model for hydrogen AAEM fuel cell. The results showed that the humidification of cathode is more important than anode, and the liquid water supply from cathode flow channel positively affect the performance.

As shown in Fig. 1, at the interface of different layers, for example, the interface of catalyst layer (CL)/micro-porous layer (MPL) or MPL/gas diffusion layer (GDL), the porosity, permeability and wettability are all different on both sides, and such interfacial effect leads to sudden change of liquid water volume fraction across the interface. It explains the role of MPL in affecting the two-phase transport. For PEM fuel cell, both experiments [17,18] and mathematical models [19,20] showed that MPL can act as liquid barrier, improving the water removal and mass transport, especially at high

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Nomenclature

A	activity
A	area (m^2)
C	molar concentration (mol m^{-3})
C_p	specific heat, J kg^{-1} K^{-1}
D	mass diffusivity (m^2 s^{-1})
E	potential (V)
EW	equivalent weight of the membrane (kg mol^{-1})
F	Faraday's constant (96485.0 C mol^{-1})
H	latent heat (J mol^{-1})
H	height (m)
I	current density (A m^{-2})
J	reaction rate (A m^{-3})
K	relative permeability (m^2); thermal conductivity (W m^{-1} K^{-1})
K	permeability (m^2)
L	length (m)
$\dot{m}$	source term of liquid pressure (kg m^{-3} s^{-1})
M	molecular weight (kg mol^{-1})
n_d	electro-osmotic drag coefficient
N	flux (mol m^{-2} s^{-1})
P	pressure (Pa)
R	universal gas constant (8.314 J K^{-1} mol^{-1})
S	liquid saturation; entropy (J mol^{-1} K^{-1})
S	source term (kg m^{-3} s^{-1}; kg m^{-2} s^{-2}; mol m^{-3} s^{-1})
T	temperature (K)
U	velocity (m s^{-1})
V	voltage (V)
W	width (m)
Y	mass fraction

Greek letters

A	kinetic transfer coefficient
γ	water phase change rate (s^{-1})
α	kinetic transfer coefficient
γ	water phase change rate (s^{-1})
δ	thickness (m)
ε	porosity
η	voltage loss (V)
θ	contact angle (°)
λ	water content in ionomer
μ	dynamic viscosity (kg m^{-1} s^{-1})
ξ	stoichiometric ratio
ρ	density (kg m^{-3})
σ	conductivity (S m^{-1}); surface tension coefficient (N m^{-1})
ϕ	potential (V); average gas relative humidity
χ	mass flux (kg m^{-2} s^{-1})

Subscripts and superscripts

A	anode
Act	active area
Aver	average
ACL	anode catalyst layer
C	cathode; capillary
Cell	fuel cell
Ch	channel
Cond	condensation
CCL	cathode catalyst layer
CL	catalyst layer
GDL	gas diffusion layer
Eff	effective
Ele	electric
Evap	evaporation
G	gas phase
h_2	hydrogen
h_2o	water
HOR	hydrogen oxidization reaction
In	inlet
L	liquid phase
M	membrane
Mw	membrane water
MPL	micro-porous layer
o_2	oxygen
ohm	ohmic
ORR	oxygen reduction reaction
Ref	reference
Rib	rib
S	solid electrode
Sat	saturation
Total	total
T	temperature
U	phase change
V_s	electric potential in the solid electrode
V_m	ionic potential in the membrane electrolyte
W	water
Wv	water vapor

current densities. For modeling such interfacial effect, liquid pressure should be continuous across the interfaces rather than liquid water volume fraction [21]. However, except one 2D model for DMFC [21], most of the previous models for hydrogen AAEM fuel cell assumed continuous liquid water volume fraction across the interfaces, and such interfacial effect was neglected.

In this study, a whole-cell 3D multiphase non-isothermal model is developed for hydrogen AAEM fuel cell, to study the effect of MPL and other important operating or design parameters on the cell performance and water transport, taking into all the essential transport and electrochemical phenomena, as well as the liquid saturation jump between two adjacent porous layers.

2. Model formulation

2.1. Physical problem

The 3D computational domain includes all the typical components of a hydrogen AAEM fuel cell: anode rib, anode flow channel (AFC), anode GDL (ADL), anode MPL (AMPL), anode CL (ACL), A201 membrane (Tokuyama Corporation), CCL, cathode MPL (CMPL), cathode GDL (CDL), cathode flow channel (CFC) and cathode rib (Fig. 1). To accelerate the convergence speed, only half rib and channel from the entire cell is included in the computational domain, due to the lateral symmetry with respect to the middle point along the channel width. The species flux along the negative Y direction (from anode to cathode) is defined to be positive. The basic model parameters are given in Table 1. The numerical model is formulated based on appropriate assumptions to simplify the