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Effect of electrode variable contact angle on the performance and transport characteristics of passive direct methanol fuel cells

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ABSTRACT

In this study, a multiphase passive direct methanol fuel cell (DMFC) model is developed to study the effect of micro porous layer (MPL) insertion, and the variable contact angle effects due to the different fabrication processes of diffusion layer (DL) and MPL are also investigated in details. It is found that with the contact angle increasing along the flow direction of methanol in anode DL (ADL), the liquid always needs to flow from a more hydrophilic region to a more hydrophobic region, leading to less methanol crossover. A higher ADL contact angle generally leads to more methanol crossover, although it increases the flow resistance at the inlet, the mass transport resistance at the DL/MPL interface is reduced, and the capillary driven flow is also enhanced inside the DL. However, since MPL is often a very thin layer compared with GDL, it could act as a mass transfer barrier mainly because of the contact angle differences across the MPL/DL and MPL/CL interfaces, which is the dominating factor determining the MPL function. The results also shed the light on the development of novel electrode with variable contact angle based on different fabrication processes.

Introduction

Passive direct methanol fuel cell (DMFC), a new kind of clean-energy power source, has extensive application prospects in portable and mobile devices because of its zero/low emission, high energy density, simple design and other favorable characteristics [1–3]. However, some technical challenges still remain for passive DMFCs, such as methanol and water crossover [4–6], electrode flooding [7], and difficulty in use of highly concentrated methanol feed [8]. As a result, understanding the multiphase transport characteristics with different cell designs and operating conditions becomes critically important.

Early designs of single passive DMFCs typically have a five-layer membrane electrode assembly (MEA) structure,

Nomenclature

a	water activity
A	specific interfacial area, m^{-1}
C	molar concentration (mol m^{-3}); gas constant
D	mass diffusivity, m^2 s^{-1}
E	potential (V); effective activation energy, J mol^{-1}
E_{cell}	cell voltage, V
E_r	thermodynamic equilibrium voltage, V
EW	equivalent weight of the membrane, kg mol^{-1}
F	Faraday's constant, 96485.0C mol^{-1}
H	Henry's constant
h	interfacial transfer rate constant (m s^{-1}), latent heat, J kg^{-1}
I	current density, A m^{-2}
j	reaction rate, A m^{-3}
K	permeability of porous material, m^2
k	thermal conductivity, Wm^{-1}K^{-1}
k_r	relative permeability
M	molecular weight, kg mol^{-1}
N	flux, mol m^{-2} s^{-1}
n_d	electro-osmotic drag coefficient
P	pressure, Pa
q	liquid water flux, mol m^{-2} s^{-1}
R	universal gas constant, 8.314 J K^{-1} mol^{-1}
s	volume fraction; entropy, J mol^{-1} K^{-1}
S	standard entropy R$^-$(J kg^{-1}), source term, kg m^{-3} s^{-1}, mol m^{-3} s^{-1}
T	temperature, K
V	partial molar volume, m^3 mol^{-1}
x	position or coordinate, m
y	position or coordinate, m

Greek letters

α	kinetic transfer coefficient
γ	reaction order
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}
ρ	density, kg m^{-3}
κ	ionic conductivity of membrane, Ω^{-1} m^{-1}
σ	surface tension coefficient, N m^{-1}
σ_s	electric conductivity, Ω^{-1} m^{-1}
Φ	potential, V

Subscripts and superscripts

a	anode
ADL	anode diffusion layer
AMPL	anode micro-porous layer
bub	carbon dioxide bubble
c	cathode, capillary
CL	catalyst layer (anode and cathode)
CO_2	carbon dioxide
diss	carbon dioxide dissolved
DL	diffusion layer (anode and cathode)
dry	dry membrane
eff	effective
ele	electrolyte
equil	equilibrium
g	gas phase
H_2O	water
in	inlet condition
ion	ionic
int	interface
l	liquid phase
LD	liquid water-dissolved water phase change
lim	limiting current density
lg	liquid and gas phase change
M	methanol
MEM	membrane
ml	methanol evaporation
MOR	the methanol oxidation reaction
mw	membrane water
MV	methanol vapor
MPL	micro-porous layer
N	Nafion
O_2	oxygen
ORR	oxygen reduction reaction
ref	reference
p	pressure
sat	saturation
T	temperature
VL	vapor–liquid water phase change
WV	water vapor

including an anode diffusion layer (ADL), an anode catalyst layer (ACL), a membrane (MEM), a cathode catalyst layer (CCL), and a cathode diffusion layer (CDL). The effects of operating and design parameters on the performance of passive DMFCs were investigated experimentally by researchers. Chen et al. [9,10] showed that by using porous metal foams rather than the conventional perforated-plates as the flow field and current collector, the performance of their passive DMFCs could be improved. Yang et al. [11] conducted surface treatment on SS316L metal bipolar plates, and showed that these bipolar plates are suitable in both anode and cathode environments of passive DMFCs. Gholami et al. [12] found that using non-uniform parallel channels is better than uniform, and one of the reasons is the improvement of CO_2 removal. Chen et al. [13] investigated the effects of cell orientation on the fuel utilization efficiency and performance, the different membranes were tested [14,15]; and researchers also experimentally studied the effects of mass transport resistances in anode and cathode [16–18], as well as the design parameters of catalyst layer [19–21]. The transient behaviors were reported by experimental studies for passive DMFCs as well [22,23]. On the other hand, mathematical models were developed to study the heat and mass transfer processes to optimize the cell design, and these models were able to compressively