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Investigation of cell orientation effect on transient operation of passive direct methanol fuel cells

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ABSTRACT

A transient model for passive direct methanol fuel cell (DMFC) is developed to investigate the effect of cell orientation and operating condition. The results show that the passive DMFC with vertical orientation has better performance than the horizontal one, except the case of high current density, because a large amount of water produced in cathode is hard to be removed in vertical orientation, which is easier for horizontal orientation due to gravity. The passive DMFC with horizontal orientation is sensitive to methanol crossover, and moderate current density or voltage is necessary to ensure high energy efficiency. The anode micro-porous layer (MPL) plays an important role in reducing the rate of methanol crossover by providing flow resistance. The MPL in cathode has a significant effect on water transport by enhancing the water back-flow from cathode to anode, which prevents water removal. Therefore, the anode MPL and cathode MPL have different effects on horizontal orientation and vertical orientation. Additionally, the size of fuel tank can improve the energy density by providing more fuel, and the effect on fuel efficiency and energy efficiency is a bit obvious in vertical orientation than horizontal orientation.

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Introduction

Direct methanol fuel cell (DMFC) has many advantages over conventional batteries: easier storage of liquid methanol fuel, higher energy density and cleaner recycling. These features make DMFC a promising power source for portable applications. The energy density of DMFC is up to 4800Whl^{-1} in theory [1], but there is still challenge to increase the fuel and energy efficiencies, which attracted great attentions. Since active DMFCs need certain ancillary devices in operation, such as

pump and fan, making it complicated and unsuitable for portable applications, passive DMFCs with simpler design and operation are often considered to be a better choice [2–4].

In a passive liquid-feed DMFC, the fuel and oxygen supply is driven by concentration gradient (fuel supply may also be driven by gravity based on cell orientation), and design optimization is needed to ensure proper reactant delivery and product removal. Many experimental studies were carried out for this purpose to optimize the membrane thickness [5], electrode structure [6] and cell structure [7,8]. For example, Ward et al. [8] designed a tubular DMFC, and the power density was

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Nomenclature	
a	Water activity
A	Active reaction area, m ²
A _{lg}	Interfacial specific area between liquid and gas phase, m ⁻¹
C	Molar concentration, mol m ⁻³
C _g	Gas constant
C _p	Specific heat capacity, J kg ⁻¹ K ⁻¹
E	Effective activation energy, J mol ⁻¹
F	Faraday's constant
h	Height, m; heat transport coefficient, W m ⁻² K ⁻¹ ; latent heat, J kg ⁻¹ ; horizontal orientation
h _{lg}	Interfacial transfer rate constant for methanol, m ² s ⁻¹
I	Current density, A m ⁻²
I _p	Parasitic current density results from methanol crossover, A m ⁻²
j	Reaction rate, A m ⁻³ ; mass flux of reaction, kg m ⁻² s ⁻¹
K	Permeability of porous material, m ²
k	Thermal conductivity, Wm ⁻¹ K ⁻¹ ; relative permeability
k _H	Henry's constant
ṁ	Source term of liquid or gas mixture, kg m ⁻³ s ⁻¹
M	Molecular weight, kg mol ⁻¹
MOR	Methanol oxidation reaction
n	Amount of substance, mol
n _d	Electro-osmotic drag coefficient
N	Mol flux, mol m ⁻² s ⁻¹
ORR	Oxygen reduction reaction
P _c	Capillary pressure, Pa
R	Universal gas constant, 8.314 J K ⁻¹ mol ⁻¹
s	Liquid saturation
S	Source terms, mol m ⁻³ s ⁻¹ ; entropy, J mol ⁻¹ K ⁻¹
t	Time, min
T	Temperature, K
u	Velocity, m s ⁻¹
v	Vertical orientation
V	Electrical potential, V
x	Position or coordinate, m; or mole fraction
<i>Greek letters</i>	
α	Kinetic transfer coefficient
γ	Reaction order; water phase change rate, s ⁻¹
δ	Thickness of porous layers, m
ε	Porosity
η	Voltage loss, V; fuel consumption efficiency
θ	Contact angle, °
κ	Electrical conductivity, S m ⁻¹
λ	Water content in ionomer
μ	Dynamic viscosity, kg m ⁻¹ s ⁻¹
ρ	Density, kg m ⁻³
σ	Surface tension coefficient, N m ⁻¹
φ	Electrical potential, V
ω	Volume fraction of ionomer in catalyst layer
<i>Subscripts and superscripts</i>	
a	Anode
air	Air
ACL	Anode catalyst layer
ADL	Anode diffusion layer
AMPL	Anode micro-porous layer
c	Cathode
CCL	Cathode catalyst layer
CDL	Cathode diffusion layer
CMPL	Cathode micro-porous layer
ch	Channel
con	Convection
cond	Condensation
cross	Crossover
diff	Diffusion
drag	Electro-osmotic drag
ele	Electronic
equil	Equilibrium
evap	Evaporation
FT	Fuel tank
g	Gas phase
i	Components i
ion	Ionic
in	Inlet condition
l	Liquid phase
LD	Liquid water-dissolved water phase change
M	Liquid methanol
MEM	Membrane
MV	Methanol vapor
MW	Membrane water
op	Operation condition
reac	Reaction
ref	Reference
rev	Reversible
rib	Rib
ro	Room condition
sat	Saturation
vl	Vapor to liquid phase change
WV	Water vapor

significantly improved. For passive methanol supply, the methanol crossover is difficult to control and always considered to be the key to improve the fuel efficiency. Moreover, the micro-porous layer (MPL), acting as a methanol barrier in anode, is often considered to be effective in reducing the methanol crossover [9–11], and the MPL in cathode may also facilitate water transport from cathode to anode [12–14]. In addition, it was also experimentally shown that the vertical and horizontal

cell orientations may lead to significantly different operating characteristics and performance [15–19]. The multiphase transient transport processes are affected by cell orientation duo to gravity and buoyancy effects, such as the transport of CO₂ bubble driven by buoyancy [20,21]. It was also experimentally found that passive DMFC with vertical orientation has longer discharging time and higher output voltage than horizontal orientation in low current density operation [22–25].

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