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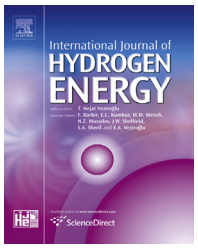

Transient analysis of passive direct methanol fuel cells with different operation and design parameters

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ABSTRACT

By developing a transient multiphase model for passive direct methanol fuel cell (DMFC), the effects of operating current density, voltage, micro-porous layer (MPL) and methanol feeding condition are comprehensively investigated for the whole operating processes (fuel tank from full to empty). It is found that for all the operating conditions, it is necessary to operate at moderate current density or voltage to limit the methanol crossover and ensure the energy conversion efficiency. The MPL in anode is needed to provide sufficient flow resistance at the MPL/gas diffusion layer (GDL) interface to improve the fuel efficiency. Although the cathode MPL can strengthen the convective transport of methanol from cathode to anode, its effect on reducing methanol crossover is less significant than the anode MPL. If the energy density is the most important factor, it is suggested to operate with sufficiently high methanol feeding concentration; and if the fuel and energy efficiencies have the priority, the methanol feeding concentration needs to be moderate. Increasing the size of fuel tank generally improves the energy density, but has negligible effect on the fuel and energy efficiencies.

Introduction

Direct methanol fuel cell (DMFC) has attracted considerable attentions in the last two decades due to its advantages of high energy density and design flexibility, which makes it suitable as portable power sources [1–3]. Theoretically, the energy density of methanol is 4800 Wh l^{-1}, which is four times of Li-ion battery (1200 Wh l^{-1}) [4].

One of the major problems hindering the commercialization of DMFC is methanol crossover: methanol moves from anode to cathode, lowering both the energy and fuel efficiencies [5–9]. Low concentration methanol solution is often used to reduce the methanol crossover, but the energy density is also decreased. Mass transport barriers were also used to reduce the methanol crossover [10–13]. For example, Casalegno et al. [10] proposed a nanostructured Pb barrier on

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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}
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, W m^{-1} K^{-1}; relative permeability
k_H	Henry's constant
$\dot{m}$	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	electrical potential, V
x	position or coordinate, m; or mole fraction

Greek letters

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

Subscripts and superscripts

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
0	intrinsic value, reference

membrane to reduce the methanol crossover, and performed experimental measurements to validate this idea. However, using a mass transport barrier may also increase the mass transport loss. Therefore, design optimization, especially the electrode design, is critically important, which requires comprehensive understanding of the multiphase transport processes.

Since active liquid-feed DMFCs require auxiliary components, which increase the system size and cost, and decrease the overall efficiency [14–18], passive design operating at ambient temperature is often considered to be suitable for portable applications [19–21] For passive DMFCs, the stored fuel is continuously consumed, and the methanol feeding condition changes during operation, in this case, transient analysis of the whole operation processes from full of methanol to empty is needed.

Experimental studies on the transient behaviors of DMFCs have been carried out [22–27]. Lai et al. [22] conducted in-situ