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Nonlinear dynamic mechanism modeling of a polymer electrolyte membrane fuel cell with dead-ended anode considering mass transport and actuator properties

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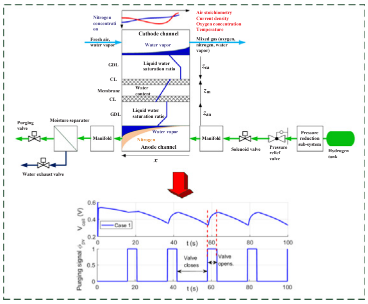
HIGHLIGHTS

- A nonlinear dynamic model based on mass transport of a fuel cell is proposed.
- Gas permeance and liquid water saturation ratio are emphasized.
- Interaction of periphery components and fuel cell are explained in details.
- The procedure of how a purging valve affects the cell voltage is revealed.

GRAPHICAL ABSTRACT



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ABSTRACT

A dead-ended anode (DEA) has advantages such as simple structure, high reliability, and low price, and is widely utilized in polymer electrolyte membrane fuel cell (PEMFC) systems. Empirical parameters are commonly adopted in control-oriented models for such systems, and detailed information about mass transport processes is usually not available. Such models are neither helpful for understanding the internal processes within fuel cells, nor for designing control algorithms to improve system performance. A control-oriented model considering the mass transport processes and actuator properties is still lacking. This paper proposes a nonlinear dynamic mechanism model for the DEA system that can describe the dynamic voltage drop during water flooding with a large current density. The properties of the major components are explained in details, and the procedure of how the purging valves affects the mass transport and cell voltage is revealed quantitatively. The relationship between the minimum cell voltage and purging operations is summarized. The results show that (1) the proposed model can capture the stable and dynamic properties of a fuel cell with a DEA, (2) the cell voltage loss during closing of the purging valve is mainly caused by a decrease in oxygen and hydrogen partial pressures on the catalyst layers and an increase in the liquid water saturation ratio in the gas diffusion layers (GDLs); (3) the most important internal states that affect the stack voltage during purging is the liquid water saturation ratio in the GDLs.

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Nomenclature

Abbreviations

CFD	computational fluid dynamic
CL	catalyst layer
DEA	dead-ended anode
ECSA	electrochemical surface area
FTA	flow-through anode
GDL	gas diffusion layer
HRA	hydrogen recirculation anode
MEA	membrane electrolyte assembly
PDE	partial differential equation
PEMFC	polymer electrolyte membrane fuel cell
PV	purging valve

Subscripts

a	anode
an	anode
avg	average
c	cathode
cell	a single fuel cell
ch	channel
chn	channel
cri	critical value
d	electro-osmotic drag effect
e	evaporation
evap	evaporation
em	exhaust manifolds
fc	fuel cell stack
g	gas OR GDL
gdl	gas diffusion layer
gen	generation
gout	out of the channel
h2	hydrogen
l	liquid
leak	leakage
liq	liquid water
lw	liquid water
m	membrane
n	internal fuel crossover through the membrane
nt	Nernst
n2	nitrogen
ohm	ohmic
o2	oxygen
phase	phase change from water vapor to liquid water
ph2	hydrogen permeance through the membrane
pn2	nitrogen permeance through the membrane
po2	oxygen permeance through the menbrane
pv	purging valve
ref	reference
rf	relief valve
s	parameter related to liquid water saturation ratio
sat	saturation
sm	supply manifolds
t	effective
tg	target
vap	water vapor
v	volume OR water
w	water
0	standard state OR standard value OR index
1	index OR downstream gas of a valve
2	index OR upstream gas of a valve
3, 4, 5, 6	index

Superscripts

an	anode
ca	cathode
cell	a single fuel cell
int	interface of CL and GDL
m	membrane
ref	reference
rf	relief valve
pt	platinum
v	volume

Parameters and variables

a	activity
c	molar concentration, mol m^{-3}
f	fraction
h	specific heat of evaporation (J kg^{-1} K^{-1}) OR convective mass-transfer coefficient (m s^{-1})
i	current density, A cm^{-2}
k	nozzle orifice coefficient (kg (s Pa)$^{-1}$) OR gas adiabatic coefficient OR permeability coefficient OR coefficient
k_{cd}, k_{re}	structure coefficients of a relief valve
m	mass, kg
n	water drag coefficient
p	pressure, pa
r	resistivity (Ω cm)
s	liquid water saturation ratio
x	molar fraction OR molar concentration
y	mass fraction
z	coordinate axis
A	area, m^2
C_{d}	flow rate coefficient, kg m s^{-1} (J mol)$^{-0.5}$
D	mutual gas diffusivity (m^2 s^{-1}) OR water diffusion coefficient in membrane (m^2 s^{-1})
E	energy per mole, kJ mol^{-1}
F	Faraday constant, 96485.3 C mol^{-1}
H	height, m
I	current, A
J	molar flux, mol m^{-2} s^{-1}
L	thickness OR length, m
M	molar mass, kg mol^{-1}
N	number OR molar flow (mol s^{-1})
R	resistance (Ω) OR ideal gas constant (8.31 J mol^{-1} K^{-1})
RH	relative humidity
R_{m}	individual gas constant, (J kg^{-1} K^{-1})
S	source term
T	temperature, K
V	voltage (V) or volume (m^3)
W	gas flux, kg s^{-1}
α	transfer coefficient
β	net water transport coefficient
γ	pressure ratio OR electrochemical surface area per unit of volume (m^2 m^{-3})
ε	GDL porosity OR conductivity coefficient (Ω^{-1} cm^{-1})
ρ	density, kg m^{-3}
η	overpotential
λ	water content
μ	viscosity
v	gas flow velocity
ϕ	purging action signal