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Quasi-three dimensional dynamic modeling of a proton exchange membrane fuel cell with consideration of two-phase water transport through a gas diffusion layer

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ABSTRACT

Water management is one of the challenging issues for low-temperature PEMFCs (proton exchange membrane fuel cells). When liquid water is formed at the GDL (gas diffusion layer), the pathway of reactant gas can be blocked, which inhibits the electrochemical reaction of PEMFC. Thus, liquid water transport through GDL is a critical factor determining the performance of a PEMFC. In present study, quasi-three dimensional dynamic modeling of PEMFC with consideration of two-phase water transport through GDL is developed. To investigate the distributions of PEMFC characteristics, including current density, species mole fraction, and membrane hydration, the PEMFC was discretized into twenty control volumes along the anode channel. To resolve the mass and energy conservation, the PEMFC is discretized into eleven and fifteen control volumes in the perpendicular direction, respectively. The dynamic variation of PEMFC characteristics of cell voltage, overvoltage of activation and ohmic, liquid water saturation through a GDL, and oxygen concentration were captured during transient behavior.

1. Introduction

The PEMFC (proton exchange membrane fuel cell) has been regarded as a promising power generation for automotive applications [1]. Although the PEMFC has the advantages of low emissions, quick response, and fast start-up, optimal water management remains one of the primary obstacles that needs to be overcome for commercialization. The proton conductivity is decreased when the membrane is not well hydrated, which increased the ohmic overvoltage, which is eventually decreasing the net performance [2,3], Whereas when the membrane is over-hydrated, the fuel cell can be saturated with the water vapor, and the water vapor molecules over the saturated value are changed into liquid water. The liquid water remaining through a GDL (gas diffusion layer) pores can block the reactant pathway, increasing the over-potential and reducing the electro-chemical reaction rates [4]. Thus, it is crucial to achieve optimal control of the membrane hydration to avoid flooding and dehydration [5,6].

The two-phase water transport in the PEMFC channel and GDL has been analyzed by several researchers. Wang et al. developed a multiphase and multicomponent PEMFC model [7]. Mazumder and Cole developed a multiphase model and investigated the liquid water distribution in PEMFCs [8]. Berning and Djilali presented the two-phase PEMFC model which can capture the two-phase flow in the MEA (membrane electrode assembly) [9]. A two-phase transport PEMFC model was developed by You and Liu [10]. They investigated the water content and the oxygen concentration distribution in the perpendicular direction of the fuel cell. Chang et al. conducted parametric sensitivity analysis by varying the parameters of GDL permeability, GDL thickness, and catalyst loading with the one-dimensional two-phase numerical model [11]. Three-dimensional PEMFC model was developed by Wang et al. [12]. They investigated the two-phase transport in GDL and its correlation with cathode flooding. Grotsch et al. presented a reduced nonlinear dynamic two-phase PEMFC model [13]. Simple two-phase dynamic PEMFC model was developed by Mckay et al. for real-time controls [14]. Khajeh-Hosseini-Dalasm et al. investigated the effects and the time variation of liquid water formation and gas phase transport of cathode side at start-up condition by their three-dimensional transient two-phase isothermal model [15]. Zamel et al. captured the effects of liquid water presence on the transport properties of the carbon paper GDL by using the full morphology model [16]. A two-phase one-dimensional steady model has been

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Nomenclature

a	water activity [−]
A	surface area [m^2]
$\vec{B}$	species transport coefficient [ms^{-1}]
C	solid specific heat capacity [kJ kg^{-1} K^{-1}]
C_P	constant pressure gas specific heat capacity [kJ kg^{-1} K^{-1}]
C_V	constant volume gas specific heat capacity [kJ kg^{-1} K^{-1}]
$\vec{C}$	species molar concentration [kmol m^{-3}]
D	diameter [m]
D_w	diffusion coefficient of water through electrolyte [m^2 s^{-1}]
D_λ	water diffusivity in Nafion [m^2 s^{-1}]
$\vec{D}$	species diffusion coefficient through GDL [m^2 s^{-1}]
$\vec{E}$	total resistance for diffusion of species [m^3 s^{-1}]
E	activation energy [kJ $kmol^{-1}$]
F	Faraday's constant [96,485 $Cmol^{-1}$]
f	friction factor [−]
ΔG	Gibbs energy [kJ $kmol^{-1}$]
$\vec{g}$	gravity [ms^{-2}]
h	enthalpy [kJ $kmol^{-1}$]
hd	head loss [m]
ΔH	formation enthalpy [kJ $kmol^{-1}$]
i_o	exchange current density [Am^{-2}]
i	current [A]
J(s)	Leverette function [−]
$\vec{j}$	liquid water flux [$kmols^{-1}$]
j_L	limiting current density [Am^{-2}]
L	length [m]
M	molecular weight [kg $kmol^{-1}$], or equivalent weight [kg $kmol^{-1}$]
N	molar capacity, or total number of moles [kmol]
$\vec{N}$	species molar capacity [kmol]
$\dot{N}$	molar flow rate [$kmols^{-1}$]
n	electron number [−]
n_d	electro-osmotic drag coefficient [−]
P	pressure [kPa]
$\dot{Q}$	heat transfer rate [kW]
R	external load resistance [ohm], or universal gas constant [8.3145 kJ $kmol^{-1}$ K^{-1}]
$\vec{\dot{R}}$	reaction rate [$kmols^{-1}$]
Re	Reynolds number [−]
s	liquid water saturation factor [−]
Sh	Sherwood number [−]
T	temperature [K]
t	time [s], or thickness [m]
V	voltage [V], or velocity [ms^{-1}]
v	volume [m^3]
$\vec{X}$	Species mole fraction [−]

Greek letters

α	activation overpotential tuning coefficient [−]
β	ohmic overpotential tuning coefficient [−]
γ	concentration overpotential tuning coefficient [−]
ε	GDL mean porosity [−]
Φ	species diffusion flux through GDL [$kmols^{-1}$]
Ψ_{H_2O}	water diffusion flux through electrolyte [$kmols^{-1}$]
Θ_{H_2O}	electro-osmotic flux [$kmols^{-1}$]
τ	surface tension [Nm^{-1}]
θ	contact angle [°]
$\sigma_{303\ K}$	conductivity of membrane at 303 K [Scm^{-1}]
ρ	density [kg m^{-3}]
λ	membrane water content [−]
ν	kinematic viscosity [m^2 s^{-1}]
K	permeability [m^2]

Subscripts

act	activation
c	capillary
cell	fuel cell
con	concentration
d	electo-osmotic drag
eff	effective
gdl	GDL
g	gas phase
H	hydraulic
H_2	hydrogen
H_2O	water
in	in to control volume
L	limiting
l	liquid phase
latent	latent
local	local section
m	dry basis membrane
mea	membrane
Nernst	Nernst
o	standard condition
O_2	oxygen
ohm	ohmic
out	out of control volume
pore	pore
ref	reference condition
s	solid phase
sat	water saturation

developed by Liu et al. to analyze the coupled phenomena of cathode flooding and mass transport limiting for the porous cathode electrode of a PEMFC [17]. Qin et al. investigated the liquid water flooding in the cathode gas channel and its impacts on the liquid water distribution in the cathode diffusion layers by using their two-phase flow model [18]. Yin et al. developed the two-dimensional PEMFC model by adopting the pseudo-phase-equilibrium function to approximate the vapor/liquid phase equilibrium [19]. Rakhshanpouri and Rowshanzamir presented the PEMFC model to achieve the optimal water management [20]. Xing et al. developed the two-dimensional isothermal model to investigate the water transport through PEMFC [21]. And they upgrade their PEMFC model as a non-isothermal two-phase model to predict PEMFC characteristics more accurately [22]. Ferreira et al. numerically investigated the two-phase flow in an anode gas channel by using CFD (computation fluid dynamics) [23]. Most previous models can be classified as simple dynamic models and multi-dimensional models. Simple dynamic models cannot resolve the detailed phenomena occurring in the PEMFC or cannot investigate the distribution of PEMFC characteristics. Because the