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Research Paper

A three-dimensional multi-phase numerical model of DMFC utilizing Eulerian-Eulerian model

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HIGHLIGHTS

- A 3D multiphase model of DMFC is developed based on the Eulerian-Eulerian model.
- The carbon dioxide in anode channel mainly accumulates at the AFC/ADL interface.
- The carbon dioxide produced in ACL is likely to accumulate under the inlet region.
- The higher the DMFC operating temperature, the more methanol crossover.
- The higher the temperature, the less carbon dioxide in DMFC due to the dissolution.

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ABSTRACT

A three-dimensional multiphase model of DMFC (direct methanol fuel cell) is developed, in which the Eulerian-Eulerian model is adopted to treat the gas and liquid two-phase flow in channel. Meanwhile, the multiphase flow in porous electrodes is solved with the help of gas and liquid pressure conservation equations to reflect the liquid saturation jump phenomenon at two different porous electrodes (e.g. DL (diffusion layer) and CL (catalyst layer)). The effects of current density, methanol concentration and temperature on gas and liquid two-phase flow in channel and porous electrodes are investigated in detail. It is found that the carbon dioxide in anode channel gradually increases along flow direction and is mainly accumulated at the interface of anode channel and DL. Meanwhile, the carbon dioxide produced in ACL (anode catalyst layer) is likely to accumulate under the inlet region and then increases along flow direction gradually. Moreover, the higher the temperature, the more methanol crossover and the less carbon dioxide produced in DMFC because of the dissolution.

1. Introduction

Over the past decade, as a clean energy power source, DMFC (direct methanol fuel cell) has drawn considerable attention because of its lower to zero emission, higher energy density and efficiency compared to other power sources (e.g. lithium-ion battery). In general, there are two basic types of DMFC: passive and active. Passive DMFC features simpler system compared to active DMFC and therefore has been widely studied in many aspects, such as water and heat management [1–11], methanol and water crossover [4,12–15] and alkaline membrane [16].

In contrast, active DMFC exhibits higher performance and is easier to control the operation condition compared to passive DMFC, because of the utilization of liquid pumps in anode, gas compressors in cathode and other devices [17,18]. So far, the effects of operation condition (temperature, methanol concentration, anode and cathode flow rate and humidification, etc.) [8,19–23] and geometry [8,24,25] on the performance of active DMFC have been investigated in detail. Kianimanesh et al. [24] analyzed different serpentine channel widths and found that the cell performance with the narrowest channel width was the best. Almheiri and Liu [26,27] measured the methanol crossover flux and current density under the land and channel separately in an active DMFC and found that the methanol crossover flux under the land is higher than that under the channel due to the convection under the land. Casalegno et al. [28] noticed that the methanol crossover is mainly caused by the diffusion through the membrane, which is greatly affected by temperature.

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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 (96485.0 C mol^{-1})
g	gravity (kg/N)
H	Henry's constant, height (m)
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})
J	Leverette function
K	permeability of porous material (m^2)
k	thermal conductivity (W m^{-1} K^{-1})
k_r	relative permeability
L	length (m)
m	the mass flow rate (kg/s)
$\dot{m}$	mass transfer
M	molecular weight (kg mol^{-1})
N	flux (mol m^{-2} s^{-1})
n_d	electro-osmotic drag coefficient
P	pressure (Pa)
Q	flow rate (ml min^{-1}, sccm)
R	universal gas constant (8.314 J K^{-1} mol^{-1}),
R_{pq}	interaction force between phases
s	volume fraction; entropy (J mol^{-1} K^{-1})
S	standard entropy $\tilde{R}$ (J kg^{-1}), source term (kg m^{-3} s^{-1}, mol m^{-3} s^{-1})
T	temperature (K)
V	partial molar volume ($m^3 mol^{-1}$), volume fraction
W	width (m)
x	position or coordinate (m)
y	position or coordinate (m)
Y	species
z	position or coordinate (m)

Greek letters

α	volume fraction, kinetic transfer coefficient
$\vec{v}$	velocity
τ	stress-strain tensor
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
ACL	anode catalyst layer
ADL	anode diffusion layer
ADL-Int	the mesh closest the ADL/AFC interface in ADL
AFC	anode flow channel
AFC-Int	the mesh closest the AFC/ADL interface in AFC
aver	average
bp	bipolar plate
c	cathode, capillary
CCL	cathode catalyst layer
CDL	cathode diffusion layer
CDL-Int	the mesh closest the CDL/CFD interface in CDL
CFC	cathode flow channel
CFC-Int	the mesh closest the CFC/CDL interface in CFC
ch	channel
CL	catalyst layer (anode and cathode)
CO2	carbon dioxide
cond	condensation
DL	diffusion layer (anode and cathode)
dry	dry membrane
eff	effective
ele	electrolyte
equil	equilibrium
Evap	evaporation
g	gas
H2O	water
i	species
in	channel inlet
Int	interface
ion	ionic
l	liquid
LD	liquid water-dissolved water phase change
m	mass
M	methanol
MEM	membrane
MOR	methanol oxidation reaction
mw	membrane water
N	Nafion
O2	oxygen
ORR	oxygen reduction reaction
outlet	channel outlet
ref	reference
p	pressure
pq	two phase
q	phase q
sat	saturation
T	temperature
VL	vapor-liquid water phase change
WV	water vapor

In order to further improve the performance of active DMFC, a basic understanding of the gas and liquid two-phase flow in the whole DMFC is critical [29]. The visualization studies conducted by researchers showed that the carbon dioxide (CO_2) in anode channel mainly accumulates at the AFC/ADL interface, which decreases the performance of DMFC by preventing the methanol diffusion to the CL (catalyst layer). In fact, the CO_2 amount in anode channel is affected by many operating factors: methanol feed concentration [30–32], temperature [30,32], anode flow rate [30,31,33], cell direction (vertical and horizontal) [32], channel length [34], etc. Burgmann et al. [35] investigated the appearance and evolution of bubbles in serpentine and parallel channels based on time-resolved measurement and showed the progress of CO_2 bubbles formation, blockage of cross-sectional channel and removal out of channel by slug. And a similar evolutionary process of bubbles was also found by Liao et al. [30].

Moreover, given the high cost and limitations in conducting visualization experiments, model development is also a popular