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Oxygen transport resistance at gas diffusion layer – Air channel interface with film flow of water in a proton exchange membrane fuel cell

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HIGHLIGHTS

- O_2 transport resistance at a GDL-air channel interface is numerically calculated.
- The effect of liquid water films on the transport resistance is investigated.
- Correlations are provided for variations of local transport resistance.
- Correlations can be used at 20–80 °C and 0–100% relative humidity.
- This resistance is significant and needs to be considered in fuel cell modeling.

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ABSTRACT

Water present as films on the gas diffusion layer-air channel interface in a proton exchange membrane fuel cell (PEMFC) alters the oxygen transport resistance, which is expressed through Sherwood number (Sh). The effect of multiple films along the flow length on Sh is investigated through 3D and stationary simulations. The effects of air Péclet number, non-dimensional film width, length, and spacing are studied. Using the simulation results, non-dimensional correlations are developed for local Sh within a mean absolute percentage error of 9%. These correlations can be used for simulating PEMFC performance over temperature and relative humidity ranges of 20–80 °C and 0–100%, respectively. Sh on the film side can be up to 31% lower than that for a dry channel, while a film may reduce the interfacial width by up to 39%. The corresponding increase in transport resistance results in lowering the voltage by 5 and 8 mV respectively at a current density of 1.5 A cm^{-2}. However, their combined effect leads to a voltage loss of 20 mV due to this additional mass transport resistance. It is therefore important to incorporate the additional resistance introduced by the films while modeling fuel cell performance.

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) are electrochemical engines that are environmentally friendly in contrast to internal combustion engines (ICEs) that are used in automotive applications. Hydrogen is used as the fuel and water is the sole byproduct. Efficient liquid water removal is a key factor to increase the PEMFC efficiency and reduce the cost. The design of PEMFCs has been evolving to match the low cost offered by current ICEs. As a part of the PEMFC design considerations, oxygen transport resistance needs to be taken into account.

As oxygen is transported from air channels toward the cathode catalyst layer, it encounters two major transport resistances: at the interface of the gas diffusion layer (GDL) and the air channel, and the GDL itself. The transport resistance in the GDL is a function of its water saturation which has been studied through numerical models [1–4], visualization techniques [5,6], and ex-situ experiments [7,8]. The interfacial transport resistance is less investigated. It has been shown that presence of liquid water in the channels adversely affects the transport by blocking the available interfacial area [9]. The blocked interfacial area has been characterized though optical visualization of operational PEMFCs [10,11] and numerical

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Nomenclature

Abbreviations

BPP	bipolar plate
CL	catalyst layer
FD	fully developed
GDL	gas diffusion layer
ICE	internal combustion engine
MAPE	mean absolute percentage error
PEMFC	proton exchange membrane fuel cell
TPCL	triple-phase contact line

Variables

A	area
a, b, c	coefficients of correlations
C	oxygen molar concentration
$D_{\mathrm{O2\text{-}air}}$	molar oxygen diffusivity in air
$D_{\mathrm{O2\text{-}GDL}}$	molar oxygen diffusivity in the gas diffusion layer
d_{h}	hydraulic diameter
F	air drag force on a film
F_{c}	Faraday's constant
H	height
h_{M}	mass transfer coefficient
$\mathbf{I}$	identity matrix
i	current density
j	magnitude of oxygen molar flux
L	length
N	number of films in the air channel
Nu	Nusselt number
Pe	Péclet number
Po	Poiseuille number
p	air pressure
r	semi-principle axis length of an ellipsoid
R_{u}	universal gas constant
Sc	Schmidt number
Sh	Sherwood number
T	temperature
$\mathbf{u}$	velocity vector
u, v, w	velocity components
V	voltage
W	air channel width
We	Weber number
$\mathbf{x}$	spatial coordinate vector
x, y, z	spatial coordinate components
Δx	distance in the flow direction

Greek

Π	non-dimensional group
θ	droplet static contact angle
μ	dynamic viscosity of air
ξ	droplet-blocked portion of the channel cross sectional area
ρ	air mass density
σ	air–water surface tension

Subscript

∞	asymptotic value
ac	repetitive unit area under a channel and land
ad	adhesion
av	averaged
ch	channel based
D	drag force along the flow direction
eff	effective
f	film
FD	fully developed
int	interfacial
m	mean
n	droplet number in the flow direction
side	side wall of the channel
st	static contact angle
top	top wall of the channel
x	flow direction specific
wet	droplet-covered portion of the GDL-channel interface

Superscript

*	non-dimensional
T	transpose

simulations [12,13]. The flow of air and water introduces different flow patterns in the channels, including droplet on the GDL surface, slug flow, film flow and mist flow. The GDL surface covered by liquid water is not available for oxygen transport, and it changes the diffusion characteristics of oxygen into the GDL in the regions not covered by water.

The oxygen concentration drop at the GDL-air channel interface can be expressed through the Sherwood number (Sh). This resistance is not well investigated in air channels with two-phase flow as explicitly mentioned by Casalegno et al. [1]. Sh has therefore been assumed to be constant throughout the length of the air channels in simplified PEMFC performance models [14–19]. For single-phase fully developed flow in channels, Sh corresponds to the fully developed Nusselt number corresponding to the same channel cross section with equivalent heat transfer boundary conditions. However, droplets, films, and slugs exist during two-phase flow and prevent fully developed conditions. Slugs completely block the interfacial transport. Droplets and films do not completely block the air flow but alter the oxygen transport in the open areas of the GDL-channel interface. Liquid films refer to water features that do not span the entire width and height of the channel cross section. They differ from droplets by not having a spherical shape and having a length in the direction of the air flow. Koz and Kandlikar characterized Sh for the cases where the GDL-air channel interface is covered with droplets [20,21]. However, films have been recognized to occur more frequently in PEMFC air channels [10,11]. The range of conditions leading to the formation of films have been demonstrated numerically by Lorenzini-Gutierrez et al. [12] and Zhu et al. [13], and experimentally by Lee and Ito [22] and Cheah et al. [23]. This study extends the authors' earlier work on droplets to simulate the oxygen transport resistance under film flow conditions, which are more prevalent in the air channels.

The interfacial transport resistance of oxygen is numerically investigated in the presence of water films. These films are sequentially placed on alternating sides of the channel, assumed to be attached to channel surfaces and are represented as solid obstructions in single-phase air flow. The shapes of these obstructions are derived from the experimental observations of water films [22–24]. In order to ensure the presence of stationary films, a detachment analysis is performed as follows: i) Air drag forces are numerically calculated. ii) Adhesion forces are theoretically calculated. iii) The resulting drag and adhesion forces are compared. The conditions that lead to detachment are not used to characterize Sh