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Interfacial oxygen transport resistance in a proton exchange membrane fuel cell air channel with an array of water droplets

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A B S T R A C T

The oxygen (O_2) transport resistance at the gas diffusion layer (GDL)–air channel interface in a proton exchange membrane fuel cell (PEMFC) is numerically investigated. The interfacial O_2 resistance under the two-phase flow conditions is needed in modeling fuel cell performance. This work focuses on simulating the effect of water droplets on the GDL surface on the mass transfer resistance at the interface. Multiple droplets are placed at the center of channel width and spaced uniformly in the flow direction. The variation of interfacial O_2 transport resistance is characterized with the non-dimensional Sherwood number (Sh). The numerical technique is validated by comparing the fully developed Sh (in the absence of droplets) to the established values in the literature. Parametric simulations are performed for variable air Péclet number (varied due to changing superficial air velocity), non-dimensional droplet size and uniform spacing. Correlations are developed to express the Sh variation in terms of the aforementioned variables and the location in the channel. The maximum error of the correlations among numerically generated 999 data points is 11%.

1. Introduction

The performance of a proton exchange membrane fuel cell (PEMFC) is adversely affected by oxygen (O_2) concentration loss from the air flow channel to the cathode catalyst layer (CL). Oxygen transport resistance at the gas diffusion layer (GDL) and air channel interface is a non-negligible component of the O_2 concentration loss. The simplified PEMFC performance models in the available literature incorporate the O_2 resistance at the GDL–channel interface as an input parameter [1–8]. However, this parameter has been taken as a constant so far in the available literature and does not reflect variable PEMFC operating conditions and the effect of two-phase flow in the channels.

Sherwood number (Sh) is the non-dimensionalized mass transfer coefficient (h_M): $\mathrm{Sh} = h_M \times d_h/D$ where d_h and D are the hydraulic diameter and diffusivity, respectively. O_2 transport resistance is inversely proportional to the mass transfer coefficient and thereby, Sherwood number. With a constant O_2 flux at the interface, the aforementioned proportionality can also be expressed by the interfacial concentration drop which is the difference between the mean concentration at a channel cross section and the average concentration at the respective interface. The interfacial concentration drop decreases with an increase in Sherwood number. This number depends on the aspect ratio of the channel cross section, boundary conditions, and local flow conditions. Local flow conditions can be characterized at cross sections with profiles of velocity and normalized concentration by using the mean value at the respective cross section. The aforementioned profiles stop varying in the direction of flow after enough distance traveled. Variations are observed only in axes normal to the flow direction. In laminar flow conditions of internal forced convection, variations of velocity and normalized concentration spans the entire channel cross section. These conditions are called fully developed (FD). In FD sections of a channel, the heat and mass transfer analogy is applicable, and Sh is the same as the Nusselt number (Nu). Hence, established Nu values can be used as Sh in PEMFC air channels with no limitations as long as the flow is fully developed. The heat and mass transfer analogy has been utilized by several researchers for the fully developed condition [9–12]. However, Nu–Sh mapping cannot always be easily performed in an air channel since liquid water features in the channel may not allow the flow to be fully developed. Since there is no equivalent heat transfer problem that resembles two-phase flow conditions in PEMFC channels, Sh needs to be simulated for channels with two-phase flow features.

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Nomenclature

Abbreviations

BPP	bipolar plate
CL	catalyst layer
FD	fully developed
GDL	gas diffusion layer
PEMFC	proton exchange membrane fuel cell

Variables

a, b, c	coefficients of correlations
C	oxygen molar concentration
$D_{\mathrm{O2\text{-}air}}$	molar oxygen diffusivity in air
$D_{\mathrm{O2-GDL}}$	molar oxygen diffusivity in the gas diffusion layer
d_{h}	hydraulic diameter
F	air drag force on a droplet
F_{c}	Faraday's constant
g	gravitational acceleration
H	air channel height
h_{M}	mass transfer coefficient
$\mathbf{I}$	identity matrix
i	current density
j	magnitude of oxygen molar flux
L	simulated air channel length
N	number of droplets in the air channel
Nu	Nusselt number
Pe	Péclet number
Po	Poiseuille number
p	air pressure
r	droplet obstruction radius
R_{u}	universal gas constant
Sc	Schmidt number
Sh	Sherwood number
t	gas diffusion layer thickness
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
av	averaged
ch	channel based
d	droplet
eff	effective
FD	fully developed
int	interfacial
m	mean
n	droplet number in the flow direction
x	flow direction specific
wet	droplet-covered portion of the GDL–channel interface

Superscript

*	non-dimensionalized
T	transpose

Water features in the air channels can disrupt the air flow, prevent it from being fully developed, and lead to a local Sh value different than the fully developed one. Among the water features observed in PEMFC air channels, droplets are the ones that emerge initially and then they transform into more complex shapes like films or slugs [13,14]. The droplet presence in the channel has been confirmed through visual observations by earlier researchers, and therefore deserves attention for research. Among the 3D and time-dependent numerical studies on the effects of water features on cell performance [15,16], Chen et al. focused on droplets and films [16]. They showed that a droplet constricts the cross section for the air flow and leads to a local high velocity field. The higher local velocity enhances the O_2 concentration at the interface and therefore increases the local cell performance. However, the effect of the droplet on Sh variation was not included in their analysis. By characterizing Sh in the vicinity of droplets, the interfacial O_2 transport resistance can be predicted for a GDL–channel interface known to be covered with droplets. Earlier researchers have used optical visualization of PEMFCs [17–26], electrochemical sensors in the flow channels [27], ex-situ [19,28–35] and numerical studies [16,19,30,36–38] to observe or predict droplet sizes and locations on the GDL–channel interface under a given PEMFC operating condition.

The droplet emergence location along the channel width alters the local flow conditions. It is known that droplets mostly emerge from under the bipolar plate (BPP) lands (ribs) [39,40]. However, there are studies suggesting that this does not always happen. Optical visualization studies documented that the droplets can emerge in the center of the channel width [17–22]. It was hypothesized that a GDL with a smaller porosity would lead to a droplet emergence more uniformly distributed along the channel width rather than concentrated underneath the BPP lands [23]. Moreover, it was proposed to make a groove in the GDL at the channel center width and along the flow direction to create a preferential droplet emergence location and hence increase cell performance [25].

The effect of droplets on Sh was studied numerically and shown to be important in the available literature. Koz and Kandlikar simulated a single droplet in an isolated 3D air channel by using a droplet-shaped obstruction [41]. The use of an obstruction allowed the steady-state solution of single-phase air flow and mass transport equations. This obstruction was centered along the channel width and local Sh was obtained along the flow direction as droplet size and superficial air velocity was varied. The variables in their analysis were selected in such a way that the numerically obtained drag force on the obstruction did not exceed the droplet-GDL adhesion force that was experimentally obtained by Das et al. [33]. Koz and Kandlikar numerically calculated $\mathrm{Sh}_{\mathrm{FD}}$ to be 3.36 for a channel cross section of 0.40 mm × 0.70 mm. This $\mathrm{Sh}_{\mathrm{FD}}$ is significantly lower than the ones previously recommended: $\mathrm{Sh}_{\mathrm{FD}} = 5.274$ [42] (value readjusted for the characteristic length of hydraulic diameter), 6.0 [43], and 5.411 [44]. Moreover, it was shown that local Sh can be larger than $\mathrm{Sh}_{\mathrm{FD}}$ downstream of the droplet [41]. As a result, a single droplet was found to decrease the interfacial O_2 resistance, a finding that is in agreement with the results of Chen et al. [16].