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Numerical investigation of interfacial transport resistance due to water droplets in proton exchange membrane fuel cell air channels

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HIGHLIGHTS

- Interfacial oxygen resistance in an air channel is numerically calculated.
- The effect of liquid water droplets on the resistance is investigated.
- The resistance is shown to decrease with air velocity, droplet size, and number of droplets.
- Spacing between the droplets is studied for the lowest resistance.
- The analogy between heat and mass transfer is investigated for this problem.

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ABSTRACT

Oxygen transport resistance at the air flow channel and gas diffusion layer (GDL) interface is needed in modelling the performance of a proton exchange membrane fuel cell (PEMFC). This resistance is expressed through the non-dimensional Sherwood number (Sh). The effect of the presence of a droplet on Sh is studied numerically in an isolated air flow channel using a commercially available package, COMSOL Multiphysics®. A droplet is represented as a solid obstruction placed on the GDL–channel interface and centred along the channel width. The effect of a single droplet is first studied for a range of superficial mean air velocities and droplet sizes. Secondly, the effect of droplet spacing on Sh is studied through simulations of two consecutive droplets. Lastly, multiple droplets in a row are studied as a more representative case of a PEMFC air flow channel. The results show that the droplets significantly increase Sh above the fully developed value in the wake region. This enhancement increases with the number of droplets, droplet size, and superficial mean air velocity. Moreover, the analogy between mass and heat transfer is investigated by comparing Sh to the equivalent Nusselt number.

1. Introduction

The performance loss due to oxygen (O_2) transport resistance on the cathode side of a proton exchange membrane fuel cell (PEMFC) is an active area of research. The O_2 transport loss becomes more significant as the current density increases. The increased transport resistance is partly due to the increased water production rate at higher current densities. The O_2 transport resistance has a non-negligible component at the gas diffusion layer (GDL)–air flow channel (Ch) interface. It has not yet been shown how water droplets on the GDL–Ch interface affect the transport resistance.

The interfacial O_2 transport resistance can be used in simplified PEMFC performance models [1–4]. This resistance is expressed through the non-dimensional Sherwood number (Sh), which is the mass transfer equivalent of the Nusselt number (Nu) for heat transfer. For fully developed flow conditions (FD), using the heat and mass transfer analogy, Sh can be taken directly from the established values of Nu for a variety of channel cross sections and boundary conditions. It is important to match the equivalent boundary condition in the associated heat and mass transfer problems with fully developed conditions. However, the flow in a PEMFC air channel may not be fully developed for two reasons: 1) suction or injection of air at the porous GDL–Ch interface, and 2) water features disrupting the air flow in the channel.

The effect of suction/injection has been studied numerically in 2D air channels (parallel plates) [5–7]. Wang et al. simulated the cathode half of a PEMFC and reported that the suction/injection did

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Nomenclature

Abbreviations

Ch	air channel
CL	catalyst layer
FD	fully developed
GDL	gas diffusion layer
PEMFC	proton exchange membrane fuel cell

Variables

Bo	bond number
C	oxygen molar concentration
C_p	constant pressure heat capacity of air
d_h	hydraulic diameter
D_{O_2-air}	molar oxygen diffusivity in air
D_{O_2-GDL}	molar oxygen diffusivity in the gas diffusion layer
F	air drag force on a droplet
F_c	Faraday's constant
g	gravitational acceleration
h	convective transport coefficient
H	air channel height
i	current density
$\mathbf{I}$	identity matrix
j	molar flux of oxygen
k	thermal conductivity of air
L	simulated air channel length
N	droplet number in the air flow direction
Nu	Nusselt number
p	air pressure
Po	Poiseuille number
q''	heat flux
r	droplet obstruction radius
R_u	universal gas constant
Sh	Sherwood number
t	gas diffusion layer thickness
T	temperature
$\mathbf{u}$	velocity vector
u, v, w	velocity components
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

ε	thermal conductivity or species diffusivity
μ	dynamic viscosity of air
Ω	Nusselt or Sherwood number
ρ	air mass density
ψ	thermal or mass convective transport coefficient
$\overline{\psi}$	channel width averaged ψ
σ	air–water surface tension
θ	droplet static contact angle
ξ	channel cross sectional area blockage ratio by droplet

Subscript

av	flow direction averaged
d	droplet
eff	effective
FD	fully developed
m	mean
M	mass transport related
max	the maximum value from the wake of the droplet of interest
N	droplet number in the flow direction
T	thermal transport related
x	flow direction specific
wet	portion of GDL–Ch interface covered by droplet

Superscript

T	transpose

not change Sh relative to the case with no suction/injection [5]. Jeng et al. [6] also simulated the cathode side of a PEMFC and confirmed the negligible effect of air injection into the channel on Sh reported by Wang et al. [5]. Hassanzadeh et al. [7] simulated an isolated reactant channel along with the boundary conditions to mimic PEMFC conditions. They parametrically investigated the effect of air suction into the GDL. A weak dependency of Sh was found on the suction rate. In summary, the 2D numerical studies suggest that the intensity of suction/injection in a PEMFC operation leads to a minor change in Sh.

In order to study the effect of liquid water features on Sh, visual characterization of the water features is required. After characterizing the shapes, sizes, and motion of the water features, these features can be incorporated into simplified models as obstructions to single-phase flow without the need for simulating the complex two-phase flow. The liquid water present in the reactant channels can be characterized through visible-light-transparent PEMFC designs. The use of visible light provides high spatial and temporal resolution compared to other options, such as X-ray radiography, neutron radiography, and magnetic resonance imaging [8]. The two-phase flow in channels of an operational PEMFC was visualized by in-situ studies [2,8–17]. Numerical investigations aim to explain the experimentally visualized trends by parametrically analyzing the two-phase flow in 3D channels [11,19–28]. Some of the numerical studies complement their research with ex-situ experiments that introduce the liquid water into PEMFC channels through artificial injection [11,19,21,28]. Moreover, there are dedicated ex-situ studies that focus on liquid droplet dynamics [29–35]. Since liquid water comes out of the GDL in the form of a droplet first and then evolves into more complex shapes such as films and slugs (also known as plugs), this study focuses on the effect of droplets on Sh.

The Sherwood number is obtained by non-dimensionalizing the mass transfer coefficient (h_M) with diffusivity (D) and channel hydraulic diameter (d_h): $\mathrm{Sh} = h_M d_h / D$. The Sherwood number reported by Wang et al. was obtained using the channel height for two parallel plates as the characteristic length instead of the hydraulic diameter [5]. The Sherwood number calculated by Wang et al. [5] is reported here with the standard definition by using the fact that the hydraulic diameter for parallel plates is two times the channel height. Wang et al. [5], Jeng et al. [6], and Hassanzadeh et al. [7] numerically calculated Sh_{FD} as 5.274, 6.0, and 5.411, respectively, in 2D simulations. The effect of a water droplet emerging from the GDL–Ch interface on Sh was first investigated by Koz and Kandlikar [36]. For a 3D rectangular channel with a width and height of 0.70 mm and 0.40 mm respectively, they numerically calculated $\mathrm{Sh}_{FD} = 3.36$, which is significantly lower than the reported 2D values. Simulations incorporated a water droplet on the GDL–Ch interface in the form of a droplet-shaped solid obstruction centred along the channel width. The droplet adhesion to the GDL–Ch interface was assessed by comparing the numerically calculated drag force on the obstruction against the