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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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.

Keywords:

Proton Exchange Membrane Fuel Cell; Interfacial Mass Transport; Water Film; Simulation; Sherwood number; Correlation

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
$D_{\text{O}_2\text{-air}}$	molar oxygen diffusivity in air
$D_{\text{O}_2\text{-GDL}}$	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
ζ	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

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 through optical visualization of operational PEMFCs [10,11] and numerical 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 as the film would be removed by the air flow.

The input parameters in this study are film length, width, and spacing, and inlet air velocity, which reflects the changes in current density and stoichiometry. Down-the-channel variations of Sh are reported on the side of a film and its wake and are expressed with two non-dimensional mathematical correlations. The changes in Sh are compared against the reduction of interfacial area due to film blockage. The effect of variations in Sh on local cell performance is analyzed by calculating and comparing voltage losses that correspond to various sets of input parameters at a constant current density.

2. Methodology for Numerical Simulations

2.1 Introduction to the Methodology of Numerical Simulations

Simulations were performed in a single air channel that complies with the U.S. Department of Energy performance targets [25]. Multiple film-shaped obstructions were placed on alternating sides of the channel. The shape of the obstructions was chosen to mimic experimentally observed stationary film shapes in the available literature. The rationale behind choosing stationary films is the following: Liquid films were shown to take a longer time to grow in the channel than the time to depart. Pressure readings and visualization from ex-

situ experiments by Colosqui et al. [26], Shah and Kandlikar [27], and Hellstern et al. [28] quantify the duration of attachment and motion of a water feature. For instance, Hellstern et al. showed that 19 seconds is required for a slug to form and only 3 seconds to exit the channel [28]. This experimental setup replicates in-situ conditions by placing a GDL in an acrylic channel. The water and air flows rate of $25 \mu\text{L min}^{-1}$ and 9 mL min^{-1} , respectively and correspond to approximately 3 A cm^{-2} and an air stoichiometry of 4.5. Based on the aforementioned results, the steady state simulations in the current study can help the audience predicting fuel cell performance when water films are in the stage of growth.

The growth of a water film takes seconds as shown by the results mentioned above. The air flow around the film complies with this growth very fast. The viscous diffusion time scale is calculated for the channel hydraulic diameter in this work, $d_h = 0.51 \text{ mm}$ and kinematic viscosity, $\nu = \mu/\rho = 16.253 \times 10^{-6}/0.828 = 19.629 \times 10^{-6}$. The time scale result is $t = d_h^2/\nu = 0.013 \text{ s}$. This is three orders of magnitude smaller than the growth time (19 s) of a water feature as reported by Hellstern et al.[28].

The diffusion of oxygen through these obstructions can be neglected since the diffusion resistance of liquid water films is four orders of magnitude larger than that of air: $D_{\text{O}_2\text{-H}_2\text{O}}$ and $D_{\text{O}_2\text{-air}}$ are 0.24×10^{-4} [29] and $0.31 \text{ cm}^2 \text{ s}^{-1}$ [21]. The length of a film (L_f) was defined such that when it is zero, the film transforms into a droplet on the channel side wall. A non-zero length corresponds to a droplet that is elongated in the flow direction. The width of a film (W_f) indicates the largest distance that the film covers on the top channel wall along the direction of channel width. In the presence of a film, the GDL-air channel interface is partially covered and thus referred to as wet interface width (W_{wet}). The distance between the films is assumed to be uniform (Δx_f) and is measured from the closest points of two adjacent films. The inlet air velocity (u_m) reflects the imposed current density (i) and stoichiometry.

The simulations numerically calculate the local Sh profile in the vicinity of films. Temperature changes are minimal in the vicinity of the film compared to the entire electrochemically active area length. This allows a given simulation to use a constant temperature for the air properties in the governing equations. The effect of temperature on Sh was investigated by conducting simulations at different air temperatures. Firstly, Sh correlations were developed at a temperature (T) and relative humidity (RH) of 80°C and 100%, respectively. Secondly, the correlations were tested against simulation results at 20°C and 0% RH in Section 3.4.4.

Fully humidified air properties of mass density (ρ) and dynamic viscosity (μ) were calculated with the correlations provided by Tsilingiris [30]. Temperature is input in $^\circ\text{C}$.

$$\rho = 1.293 - 5.538 \times 10^{-3}T + 3.860 \times 10^{-5}T^2 - 5.254 \times 10^{-7}T^3 \quad (1)$$

$$\mu = 1.716 \times 10^{-5} + 4.722 \times 10^{-8}T - 3.663 \times 10^{-10}T^2 + 1.873 \times 10^{-12}T^3 - 8.050 \times 10^{-14}T^4 \quad (2)$$

Oxygen diffusivity in the air ($D_{O_2\text{-air}}$) was approximated with Wilke's formula [31] by averaging component diffusivities with respect to their molar fractions (ω).

$$D_{O_2\text{-air}} = \frac{1-\omega_{O_2}}{\frac{\omega_{N_2}}{D_{O_2-N_2}} + \frac{\omega_{H_2O}}{D_{O_2-H_2O}}} \quad (3)$$

For fully humidified air, the molar fraction of vapor in air is $\omega_{H_2O} = p_{H_2O, \text{sat}}/p_{\text{air}}$. This was calculated based on the vapor saturation pressure formula below provided by Mench [32]. The temperature is in the unit of °C. The remaining dry air was assumed to have an oxygen – nitrogen ratio of 21 – 79 %, respectively.

$$p_{\text{sat}} = -2846.4 + 411.24T - 10.554T^2 + 0.16636T^3 \text{ [Pa]} \quad (4)$$

The diffusivity correlation for air components is provided by Fuller et al. [33]. The units for temperature (T), molecular weight (M), and pressure (p) are K, g mol⁻¹, and atm, respectively. Diffusion volumes of simple molecules (v) are provided in the same article [33].

$$D_{AB} = \frac{10^{-3}T^{1.75}\left(\frac{1}{M_A} + \frac{1}{M_B}\right)^{0.5}}{p[v_A^{1/3} + v_B^{1/3}]^2} \text{ [cm}^2 \text{ s}^{-1}] \quad (5)$$

With the aforementioned air properties, Schmidt number ($Sc = \mu \rho^{-1} D_{O_2\text{-air}}^{-1}$) was calculated. When simulating the effect of temperature, Sc was varied to represent changes in temperature and other non-dimensional input parameters were kept constant.

The density (ρ) and dynamic viscosity (μ) of the air and the diffusivity of oxygen in the air ($D_{O_2\text{-air}}$) were kept constant at 0.828 kg m⁻³, 16.253 μPa s, and 0.310 cm² s⁻¹, respectively for the simulations that led to the correlations. The input parameters were non-dimensionalized with the hydraulic diameter of the channel, 0.51 mm. The film width and length and the inlet air velocity were expressed as non-dimensional film width (W_f^*) and length (L_f^*) and Péclet number (Pe), respectively. The air properties (ρ , μ , and $D_{O_2\text{-air}}$) were expressed as the Schmidt number ($Sc = \mu \rho^{-1} D_{O_2\text{-air}}^{-1}$).

2.2 Geometry

The numerical simulations were conducted in a single air channel with single-phase air flow and film-shaped obstructions referred to as films henceforth. The authors coupled the air channel with a GDL in an earlier study [34]. This coupling allowed the investigation of oxygen diffusion underneath the flow field ribs. The same Sherwood number was obtained through simulations when the air channel was simulated alone and coupled with the GDL. The authors also studied the effect droplet-induced convection through a GDL on Sh

profile and found no significant effect even at the largest possible droplet size [34]. Since the films in this study constrict channel cross section the same amount as those that were analyzed earlier, the effect of film-induced convection can be neglected. Therefore, the flow is considered to be only in the channel. Fig. 1 shows the channel and flow field (FF) dimensions. The electrochemically active area (A_{ac}) is a repeating pattern that covers the width of the GDL-air channel interface and a bipolar plate land (rib) width. The land width (W_{land}), channel width (W_{ch}), and channel height (H_{ch}) were selected to be 0.50 mm, 0.70 mm, and 0.40 mm, respectively [25]. The active area length (L_{ac}) was selected as 183.00 mm [25] for calculating the superficial air velocity that corresponds to a current density.

Fig. 1a shows multiple films placed in a row and on alternating sides ($y_f = 0$ and $y_f = W_{ch}$) in the channel. These films are numbered in the flow direction with the variable, n . The Sh profile changes in the flow direction and ultimately merges into a repeating pattern after a certain number of films. The total number of films (N) was selected to be large enough for the results not to differ significantly in the flow direction by the last film. It was found that the required number of films for the Sh profile to merge into a repeating pattern is dependent on Δx_f . Hence, N was selected based on each value of Δx_f .

Both single and multiple film scenarios were studied. A film was represented by a combination of the following basic geometrical shapes: spheres, cylinders, and a rectangular prism. This convention represents the top ($-z$ direction) and cross sectional ($-x$ direction) views of air channels observed by Gopalan and Kandlikar [24], Lee and Ito [22], and Cheah et al. [23]. This geometry was subtracted from the rectangular-prism-shaped channel to simulate single-phase air flow.

Fig. 1a depicts the building components of a film with dotted lines. W_f was varied from 0.20 to 0.50 mm (corresponding to non-dimensional values of 0.39 to 0.98, respectively). When the film length (L_f) is zero, the film becomes a droplet at the channel corner. In this work, droplets emerging from channel corners are also analyzed as a starting point for films and are referred to as films with zero length. Non-zero L_f values were 1.00, 2.00, and 5.00 mm (non-dimensionally: 1.96, 3.92, and 9.80, respectively). The uniform spacing between the films (Δx_f) were 1.00, 2.00, and 5.00 mm (non-dimensionally: 1.96, 3.92, and 9.80, respectively).

The spheres and the cylinder which were in contact with the GDL-air channel interface were truncated in such a way that the apparent static contact angle ($\theta_{st,GDL}$) is 147° . The GDL contact angle was selected as a representative value of the GDLs characterized by Gopalan and Kandlikar [35] and Das et al. [36]. Graphite was selected as the channel wall material. The advancing and receding contact angles on a graphite plate were measured to be 85° and 61° respectively [35]. The static contact angles on the graphite channel side ($\theta_{st,side}$) and

top walls ($\theta_{\text{st,top}}$) were assumed to be 90° . The static angles were used to generate the film-shaped obstructions. The advancing and receding angles were used to calculate the contribution of side and top walls to the film adhesion force. The film width and the aforementioned static contact angle on the GDL leads to an interfacial width coverage ($W_{\text{wet}}(x)$) as defined in Eq. (6).

$$W_{\text{wet}}(x) = \begin{cases} (x_{f,n} \leq x \leq x_{f,n} + L_f) \rightarrow W_f \cos\left(\pi \frac{\theta_{\text{st,GDL}} - 90^\circ}{180}\right) \\ \text{Else} \rightarrow 0 \end{cases} \quad (6)$$

2.3 Post-Processing and Non-Dimensionalization

The objective of this work is to find the oxygen concentration drop (ΔC) for a given magnitude of oxygen flux (j) at the GDL-air channel interface. Non-dimensional variables were used to reduce the number of simulations and obtain correlations that are applicable to a wider range of conditions. Buckingham Pi Theorem [37] was used to obtain the following non-dimensional variables: Schmidt number ($Sc = \mu \rho^{-1} D_{\text{O}_2\text{-air}}^{-1}$), non-dimensional film width ($W_f^* = W_f d_h^{-1}$), non-dimensional film length ($L_f^* = L_f d_h^{-1}$), non-dimensional film spacing ($\Delta x_f^* = \Delta x_f d_h^{-1}$), Péclet number ($Pe = d_h u_m D_{\text{O}_2\text{-air}}^{-1}$), and Sherwood number ($Sh = j d_h \Delta C^{-1} D_{\text{O}_2\text{-air}}^{-1}$).

Sh was shown to be a function of Pe, L_f^* , W_f^* , Δx_f^* , and Sc. As long as these parameters are constant, simulating Sh at different current densities always leads to the same result. Mapping current densities to Péclet numbers was performed in this study to obtain a parametric range of Pe. As a result, the users of correlations can obtain the Sh by using Péclet number first and then, find the oxygen concentration drop at the desired local current density.

For the numerical evaluation of Sh, the local oxygen transport resistance is calculated at every point on the GDL-air channel interface. For a given j , the corresponding ΔC , is the difference between the O_2 concentration at the interface ($C_{\text{int}} = C(z=0)$) and the mean value at a channel cross section (C_m). This resistance is expressed with the mass transfer coefficient (h_M).

$$h_M(x, y) = j \Delta C^{-1} = j(C_m - C_{\text{int}})^{-1} \quad (7)$$

$$C_m(x) = \frac{\int_{\text{cross section}}^{\text{Channel}} C u dA}{\int_{\text{cross section}}^{\text{Channel}} u dA} \quad (8)$$

In simulations, h_M is zero at the portion of the GDL-channel interface that is covered by a film: $W_{\text{wet}}(x)$. Eq. (9) presents an effective mass transfer coefficient ($h_{M,\text{eff}}$). This variable assigns a value of h_M everywhere on the interface ($z = 0$).

$$h_{M,\text{eff}}(x, y) = \begin{cases} \text{Dry Interface} \rightarrow h_M \\ \text{Wet Interface} \rightarrow 0 \end{cases} \quad (9)$$

In Eq. (10), the variations of $h_{M,\text{eff}}(x,y)$ were averaged along the dry GDL-channel interface width ($W_{\text{ch}} - W_{\text{wet}}(x)$) into the dry-region-averaged mass transfer coefficient ($\overline{h_M}(x)$). The resulting variable only varies in the flow direction.

$$\overline{h_M}(x) = \frac{1}{W_{\text{ch}} - W_{\text{wet}}} \int_{y=0}^{W_{\text{ch}}} h_{M,\text{eff}} dy \quad (10)$$

The dependency of $\overline{h_M}$ on d_h and $D_{\text{O}_2\text{-air}}$ was eliminated with the use of Sherwood number ($\text{Sh} = \overline{h_M} d_h D_{\text{O}_2\text{-air}}^{-1}$). The loss of interfacial area due to coverage by water features leads to an increase in the net mass transport resistance which has been integrated into Sh. A variation of Sh is defined as the effective Sh (Sh_{eff}) which can be related to Sh as shown in Eq. (11). For simplified PEMFC performance models that incorporate the effects of films, the use of Sh_{eff} instead of Sh is important to account for the loss of interfacial area.

$$\text{Sh}_{\text{eff}}(x) = \text{Sh}(x) [W_{\text{ch}} - W_{\text{wet}}(x)] W_{\text{ch}}^{-1} \quad (11)$$

2.4 Governing Equations for the Numerical Model

In this numerical study, convective mass transport was modeled with a steady-state and 3D formulation of the governing equations. Air was assumed to be incompressible. Continuity and Navier-Stokes equations are shown in Eqs. (12) and (13) respectively and were solved simultaneously. Following their solution, the oxygen transport was simulated by the advection-diffusion equation as presented in Eq. (14). The diffusive component was modeled by Fick's law, a simplified formulation of the Maxwell-Stefan equation. This simplification is justifiable for a dilute species as stated by Krishna and Wesselingh [38]. Since oxygen had a molar fraction of 0.11 at the channel inlet, Fick's law could be utilized.

$$\rho \nabla \cdot \mathbf{u} = 0 \quad (12)$$

$$\rho(\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] \quad (13)$$

$$\mathbf{u} \cdot \nabla C = \nabla \cdot (D_{\text{O}_2\text{-air}} \nabla C) \quad (14)$$

In order to reduce the computational cost of the numerical solution, the entire length of the channel was divided into three sections and the resulting shorter channel sections were simulated sequentially along the flow direction. The resulting flow profiles at the exit of the first and second sections were mapped as inlet conditions for the following sections. All films were housed in the third section. The array of films was placed 5.00 mm from the section inlet. For convenience, $x = 0$ and 5.00 mm will refer to the third channel inlet and the location of the first film, respectively in the following text. This technique was verified by comparing two approaches that simulated the entire channel either as a single domain and three separate domains.

The numerical domain is meshed with tetrahedral mesh elements and boundary layer mesh elements were used on the channel walls and film boundaries to increase accuracy. The maximum mesh element size was 102.0 μm , established as a result of a mesh independency study to be presented in Section 3.1.

2.5 Boundary Conditions and the Numerical Solution Technique

The magnitude of O_2 flux into the GDL-air channel interface ($j_{\text{O}_2,\text{int}}$) is a function of i , which was assumed to be uniform over the entire active area and ranged from 0.1 to 1.5 A cm^{-2} . With Faraday's law, the magnitude of O_2 flux at the interface was calculated to be $j_{\text{O}_2,\text{int}} = 0.444 \times 10^{-2} - 6.662 \times 10^{-2} \text{ mol m}^{-2} \text{ s}^{-1}$. A uniform velocity profile was imposed at the channel inlet with the corresponding superficial air velocity (u_m). Table 1 presents the mapping from i to u_m and Pe .

Uniform O_2 concentration (3.83 mol m^{-3}) was imposed at the inlet. Zero gauge pressure was imposed at the outlet. At this boundary, species transport took place only by advection. No-slip boundary condition was imposed at the channel side walls, top wall, and film surfaces. Since the O_2 transport through the film is negligible compared to that at the GDL-air channel interface, the O_2 flux (j_{O_2}) was imposed to be zero on the film boundary. The side top walls of the channel had zero j_{O_2} .

The numerical model was solved with COMSOL Multiphysics® 4.3, utilizing the iterative solver, Generalized Minimum Residual Method (GMRES), which utilizes a geometric multigrid scheme. The unknowns of $\mathbf{u}$ and C were represented with second-order shape functions while p was represented with a first-order one. Automatically scaled error residuals were required to converge to 10^{-6} .

2.6 Film Adhesion Analysis

Fig. 2 shows a typical film viewed from two orthonormal axes: z (top of the channel) and y (side of the channel). The triple-phase contact lines (TPCLs) are shown with solid lines on the top and side channel walls in Figs. 2a and 2b, respectively. TPCL on the GDL is shown with a line of dashes and dots in Fig. 2a. The length of the film (L_f) was assigned to be zero to represent the earlier stages of water emergence from the GDL (not shown in Fig. 2). For curved TPCLs, two angular position variables were defined (α_y and α_z) and were measured between the normal to the TPCL and flow directions. As the convention, the angle $\alpha = 0$ is directed towards the upstream of the air flow.

The adhesion force of a film (F_{ad}) has components from the GDL ($F_{\text{ad,GDL}}$), channel side wall ($F_{\text{ad,side}}$) and top wall ($F_{\text{ad,top}}$): $F_{\text{ad}} = F_{\text{ad,GDL}} + F_{\text{ad,side}} + F_{\text{ad,top}}$. TPCLs on the GDL at the positions of $x < x_f$ and $x > x_f + L_f$, correspond to the footprint of truncated spheres and hence, are the split components of a droplet footprint. The

GDL component of the adhesion force was calculated through the adhesion force per unit footprint perimeter which is provided by Das et al. [36]. They experimentally obtained this force for aged Sigracet (SGL) 24BA (5% Teflon loading) and 24DA (20% Teflon loading) as 22 and 17 $\mu\text{N mm}^{-1}$, respectively [36]. An average value of 20 $\mu\text{N mm}^{-1}$ was used in the adhesion force calculations.

The adhesion force due to the air channel side wall and top wall can be calculated using the contact angle hysteresis obtained for the wall material. The contact angles on the channel walls range from θ_{rec} to θ_{st} as α varies from 0 to $\pi/2$. For values of $\pi/2 \leq \alpha \leq \pi$, θ varies from θ_{st} to θ_{adv} . Utilizing Eqs. (15) – (18), contributions to the adhesion force from the aforementioned walls can be calculated at curved TPCLs. Eqs. (16) and (127) assume a linear variation from the advancing to receding contact angle points at the TPCL. For straight TPCLs that are normal to the x axis, the entire line takes either an advancing or a receding contact angle value.

$$F_{\text{ad}} = \sigma W_f \int_{\alpha=0}^{\pi} \cos \alpha \cos \theta d\alpha \quad (15)$$

$$\theta = \theta_{\text{ramp}}[\theta_{\text{adv}} - \theta_{\text{rec}}] + \theta_{\text{rec}} \quad (16)$$

$$\theta_{\text{ramp}} = \alpha/\pi \quad (17)$$

$$\alpha = \begin{cases} (x \leq x_f) \rightarrow \cos^{-1}[(x_f - x)/W_f] \\ [x_f < x < (x_f + L_f)] \rightarrow \pi/2 \\ [x \geq (x_f + L_f)] \rightarrow \cos^{-1}[(x_f + L_f - x)/W_f] \end{cases} \quad (18)$$

The integral in Eq. (15) needs to be calculated at each curved TPCL as shown in Fig. 2, except the ones on the GDL. The contributions to adhesion force from the side and top walls, and the GDL are presented in Table 2. At the smallest film width, the side walls contribute the most to the adhesion force. The GDL provides the highest contribution for $W_f \geq 0.25$ mm. These contributions are independent of the film length.

Table 3 presents numerically calculated drag forces on a film ($F_{\text{D},f}$) with zero-length ($L_f = 0$) at variable width (W_f) and superficial air velocities (u_m). For a given W_f , u_m was increased incrementally until detachment was achieved. The value of u_m at which detachment was achieved for a given W_f was used as the maximum value for any film length. As films elongate ($L_f > 0$), the drag has an additional contribution from the shear applied to the side of the film. Non-zero length films were assumed to detach when their respective zero-length analysis predicted the detachment.

Utilizing the aforementioned detachment prediction, each film length had 58 simulated cases as shown in Table 3. As there were 4 film lengths simulated, a total of 232 simulations were performed. For building Sh correlations, combinations of W_f - u_m were selected to match the attachment cases presented for zero film lengths in Table 3. A total of 208 data points were used to build the correlations. Table 4 presents the W_f - u_m combinations that were analyzed for multiple film scenarios. There are 21 cases in this table. A case in Table 4

was repeated for every combination of 4 film lengths and 3 film spacing values. This led to 252 multiple film simulations.

3. Results

3.1 Mesh and Geometry Independency of Films

A mesh independency study was conducted for a single, zero-length film with the respective parameters of W_f and u_m : 0.50 mm and 10.59 m s^{-1} . A zero-length film was preferred as it causes the largest flow disruption and hence, the strongest requirement for a high quality mesh. Comparisons were made between two mesh cases with maximum mesh element sizes of 68.6 and 102.0 μm . The drag forces on the film ($F_{D,f}$) showed no significant variance between the two mesh cases. Local Sh profiles were also compared and no detectable difference was found.. Therefore, the mesh with a maximum element size of 102.0 μm was used for all film simulations as it was less computationally demanding. In this mesh configuration, the fully developed channel Sh ($Sh_{FD,ch} = 3.35$) and Pouiselle number ($Po_{FD,ch} = 15.12$), match with well-established values in the literature as presented earlier [21].

Following the mesh independency verification, the effect of film entrance type on local Sh was investigated. Dimensions of r_x and r_y that were shown in Fig. 1 defines the entrance type which helps to establish a convention for defining the film shape. In one geometrical configuration, referred to as “Sharp Entrance”, r_x and r_y were selected to be equal and are shown in Fig. 1a. Another geometrical configuration, referred to as “Smooth Entrance”, represents physical conditions of large air velocities with $r_x = 2r_y$. In both configurations, W_f is equal to r_y which was kept t at 0.50 mm with an air velocity of 10.59 m s^{-1} . The rationale behind selecting high values of u_m and W_f was obtaining a high dependency of local Sh on the film entrance type.

Fig. 3 shows the effect of entrance types as described in the paragraph above on Sh. At the location where a film reaches its full width, local Sh values reach their respective maxima. After a distance of W_f downstream of the Sh peak, the maximum difference between local Sh values remains within 10%. Hence, the effect of film entrance type on Sh can be neglected in this study. For the convenience of defining the film geometry, “Sharp Entrance” convention was selected to be used for the simulations.

3.2 Zero-Length Films

The first set of simulations was performed for zero length films. Figs. 4a and 4b show cases with an absence and presence of Sh overshoot, respectively, the presence of which is dependent on Pe and W_f^* . In the film wake, a Sh minimum ($Sh_{\min}$) is observed followed by, in certain cases, a local maximum ($Sh_{\max}$). When within 1% range, Sh was assumed to converge to $Sh_{FD,ch}$.

The presence of Sh overshoot in the film wake was only seen in the shortest film length ($L_f = 0$), and at high Pe and W_f^* values. The highest $Sh_{\max}$ was 3.46 at the conditions Pe = 174.22 and $W_f^* = 0.78$. Since this value corresponds only to a 3% increase above $Sh_{FD,ch}$, the conditions that lead to Sh overshoot were post-processed without reporting $Sh_{\max}$ values.

Minimum values of Sh that are downstream of a film are always seen at a position ($x_{\min}$) in between the film (x_f) and the downstream end of the film ($x_f + W_f$). Since film-affected wake is much longer compared to W_f , $Sh_{\min}$ can be assumed to be located at the film (x_f) while generating the Sh profile from the correlations. Tables 5 and 6 respectively show normalized $Sh_{\min}$ and the distance required to converge to $Sh_{FD,ch}$ downstream of $Sh_{\min}$. Only a select number of data points are presented in the tables as they were sufficient to show the trends. The correlations to be presented will cover the entire set of data points simulated.

The values in Table 5, which range from 0.46 to 0.92, decrease with W_f^* and increase with Pe. The emboldened values indicate a Sh overshoot in the film wake as shown in Fig. 4b. These cases are the minority since the films detach before the Pe and W_f^* can become sufficiently high.

In Table 6, for conditions with no Sh overshoot, values range from 1.51 to 5.33 mm, increase with both Pe and W_f^* . The film-affected distances are many times larger than the size of the films inducing this effect. For conditions with Sh overshoot (shown with emboldened values), the distance is shortened drastically, as exemplified by the difference between Fig. 4a and 4b. The term “convergence” is used superficially to refer to the point where the Sh profile crosses $Sh_{FD,ch}$ for the first time. This crossing occurs upstream of the overshoot position. The actual convergence occurs downstream of the overshoot. However, downstream of the overshoot is not an area of interest since the overshoot is not strong enough to diverge from $Sh_{FD,ch}$ significantly.

3.3 Films with a Length Larger than Zero

Fig. 5 shows a typical Sh profile for films with lengths larger than zero. This profile has characteristic points that are shared by films with zero length: $x_{\max}$, $x_{\min}$, and x_{conv} . In addition to these shared points, there is another characteristic point specific to films with lengths larger than zero. This point indicates the Sh (Sh_{ext}) in the vicinity of film exit (x_{ext}) where film width starts tapering off to zero from W_f in the flow direction.

Sh on the side of a film exponentially decreases in the flow direction as shown in Fig. 3. If L_f is large enough, the value of Sh_{ext} can reach to a fully developed film Sh ($Sh_{FD,f}$). It is important to underline the difference between $Sh_{FD,f}$ and $Sh_{FD,ch}$. The value of $Sh_{FD,ch}$ is singular and specific to the dry channel cross section of $0.70 \text{ mm} \times 0.40 \text{ mm}$. On the contrary, the value of $Sh_{FD,f}$ is plural and varies with the cross section of the channel that is left after the partial occupancy by a film. For the aforementioned reason, $Sh_{FD,f}$ varies with the film width. Table 7 presents $Sh_{FD,f}$ as a function of W_f^* . Values of $Sh_{f,FD}$ are inversely proportional to W_f^* .

A film with non-zero length creates a strong variation of local Sh from its entrance to its exit. Comparison between Sh_{max} and Sh_{ext} can be made using the tables below. Sh_{max} is independent of film length and a function of Pe and W_f^* . Values of Sh_{max} are first normalized with the corresponding $Sh_{FD,f}$ and then presented in Table 8. The maximum value of $Sh_{max}/Sh_{FD,f}$ was obtained to be 2.25 at the conditions of $Pe = 121.91$ and $W_f^* = 0.78$.

Table 9 shows Sh_{ext} after it is normalized with the corresponding $Sh_{FD,f}$ for $L_f^* = 1.96$ ($L_f = 1.00 \text{ mm}$). Other non-tabulated Sh_{ext} results, that were obtained from other L_f^* simulations, were also used to analyze $Sh_{ext}-L_f^*$ dependency. Sh_{ext} is a function of how much the air flow is developed from the film inlet to exit. Hence, the value is dependent on Pe, W_f^* , and L_f^* . Both Pe and W_f^* increase $Sh_{ext}/Sh_{FD,f}$ while L_f^* decreases it. The largest deviation of Sh_{ext} from $Sh_{FD,f}$ is 15%, which occurs at $L_f^* = 9.80$.

Values of $Sh_{min}/Sh_{FD,ch}$ show the same dependency on Pe and W_f^* as observed in zero-length films. Values of $Sh_{min}/Sh_{FD,ch}$ either remain the same or decrease with L_f^* . When the flow is nearly fully developed on the side of a film (low Pe and low W_f^*), $Sh_{min}/Sh_{FD,ch}$ show either no difference or an insignificant difference with L_f^* . For other conditions, the larger the L_f^* value is the smaller $Sh_{min}/Sh_{FD,ch}$ becomes. The minimum $Sh_{min}/Sh_{FD,ch} = 0.39$ was obtained at conditions of $Pe = 26.16$, $W_f^* = 0.98$, and $L_f^* = 3.92$ and 9.80 . Due to this low value, the Sh convergence length in the film wake has high transport resistance.

Results reveal that Pe, W_f^* , and L_f^* positively affect the convergence length ($x_{conv}-x_f-L_f$). All the tabulated convergence lengths show that films, regardless their lengths, affect a downstream distance much longer than the respective film length. This distance can be as long as 13.48 mm for a film with $L_f^* = 9.80$ when Pe and W_f^* were 174.22 and 0.59, respectively.

3.4 Sh Correlations for Films

In this section, non-dimensional correlations of Sh are provided for the side of a film that remains exposed to air flow and the film wake. The first step to correlate Sh_{eff} is to relate Sh_{eff} and Sh by using Eqs. (6) and (11). The conditional statement in Eq. (6) outputs a non-zero W_{wet} value when down-the-channel position corresponds

to a film. The maximum variation between Sh_{eff} and Sh occurs at the largest film width with the relation of $Sh_{eff}=Sh \times 0.69$.

3.4.1 Correlations of Sh on the Side of a Film

Eq. (19) provides the correlation for $Sh_{FD,f}$. Local Sh on the side of a film is expressed with respect to $Sh_{FD,f}$ in Eq. (20). The variation of $Sh/Sh_{FD,f}$ along the flow length resembles the Graetz problem. This resemblance allows a logarithmic correlation between the non-dimensional distance along the film ($x_{f,n}^*$) and the value of $Sh/Sh_{FD,f}$.

$$Sh_{FD,f} = 1.5234W_f^{*2} - 2.7649W_f^* + 3.5643 \quad (19)$$

Eq. (20) utilizes $x_{f,n}^*$ which is defined in Eq. (21). The coefficients a_1 and b_1 are expressed in Eq. (22). The use of Eq. (20) within the film region leads to a $Sh/Sh_{FD,f}$ value that is larger than unity at the film entrance. As $x_{f,n}^*$ grows in the flow direction, there is a value of $x_{f,n}^*$ at which $Sh/Sh_{FD,f}$ reaches to unity. For any value of $x_{f,n}^*$ further downstream, Eq. (20) should continue outputting unity. In order to ensure that the logarithmic function does not output any value lower than unity, Eq. (20) is written as a conditional statement.

$$\frac{Sh}{Sh_{FD,f}} = \begin{cases} \{[a_1 \log_{10}(x_{f,n}^*) + b_1] \leq 1\} \rightarrow a_1 \log_{10}(x_{f,n}^*) + b_1 \\ \{[a_1 \log_{10}(x_{f,n}^*) + b_1] > 1\} \rightarrow 1 \end{cases} \quad (20)$$

The non-dimensional distance, $x_{f,n}^*$ is a function n in the flow direction and Δx_f (in cases of multiple films), and L_f . The dimensional distance on the side of a film is non-dimensionalized with d_h and Pe .

$$x_{f,n}^* = [x - x_{f,1} - (n - 1)(\Delta x_f + L_f)] d_h^{-1} Pe^{-1} \quad (21)$$

$$\begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = \begin{bmatrix} a_2 & b_2 \\ a_3 & b_3 \end{bmatrix} \begin{bmatrix} Pe \\ 1 \end{bmatrix} \quad (22)$$

$$\begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} -0.0031 & 0.0005 \\ -0.2175 & -0.0528 \end{bmatrix} \begin{bmatrix} W_f^* \\ 1 \end{bmatrix} \quad (23)$$

$$\begin{bmatrix} a_3 \\ b_3 \end{bmatrix} = \begin{bmatrix} 0.004 & -0.0072 & 0.0016 \\ 0.1187 & -0.2031 & 0.9438 \end{bmatrix} \begin{bmatrix} W_f^{*2} \\ W_f^* \\ 1 \end{bmatrix} \quad (24)$$

3.4.2 Correlations of Sh in the Film Wake

Similarly to the previous section, Sh trends in the film wake resembles the Graetz problem. Local Sh is normalized with $Sh_{FD,ch}$ and then correlated to non-dimensional distance measured from the start of the film end ($x_{w,n}^*$). The logarithmic correlation between $Sh/Sh_{FD,ch}$ and $x_{w,n}^*$ is presented in Eq. (25). The definition of $x_{w,n}^*$ is provided in Eq. (26).

$$\frac{\text{Sh}}{\text{Sh}_{\text{FD, ch}}} = \begin{cases} \{[a_1 \log_{10}(x_{w,n}^*) + b_1] \leq 1\} \rightarrow a_1 \log_{10}(x_{w,n}^*) + b_1 \\ \{[a_1 \log_{10}(x_{w,n}^*) + b_1] > 1\} \rightarrow 1 \end{cases} \quad (25)$$

$$x_{w,n}^* = [x - x_{f,1} - nL_f - (n-1)\Delta x_f] d_h^{-1} \text{Pe}^{-1} \quad (26)$$

The correlations for a_2 , a_3 , b_2 , and b_3 are available for two different ranges of Pe , namely $\text{Pe} \leq 69.75$ and $\text{Pe} \geq 69.75$. The aforementioned correlations for $\text{Pe} \leq 69.75$ are presented in Eqs. (27) – (31).

$$\begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} -0.0096a_4 & 0.0009b_4 \\ 0.8926a_5 & -0.0393b_5 \end{bmatrix} \begin{bmatrix} W_f^* \\ 1 \end{bmatrix} \quad (27)$$

$$\begin{bmatrix} a_4 \\ b_4 \\ a_5 \\ b_5 \end{bmatrix} = \begin{bmatrix} 0.7083 + (5.955 - 0.7083) \exp(-1.13L_f^*) \\ 0.8889 + (81.89 - 0.8889) \exp(-1.682L_f^*) \\ 0.865 + (6.033 - 0.865) \exp(-1.345L_f^*) \\ -1.677 + (66.05 + 1.677) \exp(-1.37L_f^*) \end{bmatrix} \quad (28)$$

$$\begin{bmatrix} a_3 \\ b_3 \end{bmatrix} = \begin{bmatrix} 0.0163a_6 & -0.0282b_6 & 0.0071c_6 \\ -0.9007a_7 & 1.7209b_7 & 0.732c_7 \end{bmatrix} \begin{bmatrix} W_f^{*2} \\ W_f^* \\ 1 \end{bmatrix} \quad (29)$$

$$\begin{bmatrix} a_6 \\ b_6 \\ c_6 \end{bmatrix} = \begin{bmatrix} 0.0274 & -0.338 & 1.0138 \\ 0.0216 & -0.2722 & 1.0193 \\ 0.0222 & -0.2837 & 1.0259 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (30)$$

$$\begin{bmatrix} a_7 \\ b_7 \\ c_7 \end{bmatrix} = \begin{bmatrix} 0.0145 & -0.1445 & 1.0089 \\ 0.0103 & -0.1138 & 1.0288 \\ -0.0084 & 0.0994 & 0.9771 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (31)$$

$$\begin{bmatrix} a_2 \\ b_2 \end{bmatrix} = \begin{bmatrix} 0.0099a_4 & -0.0086b_4 & 0.0014c_4 \\ -0.701a_5 & 1.1288b_5 & -0.211c_5 \end{bmatrix} \begin{bmatrix} W_f^{*2} \\ W_f^* \\ 1 \end{bmatrix} \quad (32)$$

$$\begin{bmatrix} a_4 \\ b_4 \\ c_4 \end{bmatrix} = \begin{bmatrix} 0.0523 & -0.7199 & 1.9882 \\ 0.056 & -0.762 & 2.2791 \\ 0.0805 & -1.0929 & 3.1905 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (33)$$

$$\begin{bmatrix} a_5 \\ b_5 \\ c_5 \end{bmatrix} = \begin{bmatrix} 0.0547 & -0.7215 & 2.3618 \\ 0.0243 & -0.3001 & 1.5204 \\ 0.0262 & -0.3078 & 0.985 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (34)$$

$$\begin{bmatrix} a_3 \\ b_3 \end{bmatrix} = \begin{bmatrix} 0.0241a_6 & -0.0165b_6 & 0.0023c_6 \\ -1.6684a_7 & 1.6517b_7 & 0.7465c_7 \end{bmatrix} \begin{bmatrix} W_f^{*2} \\ W_f^* \\ 1 \end{bmatrix} \quad (35)$$

$$\begin{bmatrix} a_6 \\ b_6 \\ c_6 \end{bmatrix} = \begin{bmatrix} 0.0022 & -0.0471 & 0.3451 \\ 0.0058 & -0.0835 & 0.4747 \\ 0.0302 & -0.3991 & 1.3623 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (36)$$

$$\begin{bmatrix} a_7 \\ b_7 \\ c_7 \end{bmatrix} = \begin{bmatrix} -0.0169 & 0.2154 & -0.1135 \\ -0.0175 & 0.2492 & -0.207 \\ 0.0022 & -0.0484 & 1.5556 \end{bmatrix} \begin{bmatrix} L_f^{*2} \\ L_f^* \\ 1 \end{bmatrix} \quad (37)$$

3.4.3 Accuracy of Single-Film Sh Correlations

Fig. 6 presents a representative comparison between the numerically generated Sh and correlation-predicted Sh (Sh_{cor}) at the film wake. This film has the following configuration: $Pe = 26.16$, $W_f^* = 0.39$, and $L_f^* = 9.80$. Fig. 6a shows the superposition of Sh and Sh_{cor} plotted against the logarithm of non-dimensionalized distance in the film wake (x_w^*) as defined in Eq. (26). As Fig. 6a depicts, there is a very good agreement between the numerical data and the prediction. A quantification of the prediction accuracy is presented in Fig. 6b. This figure presents the ratio of Sh_{cor}/Sh . It can be noted that the maximum error for the prediction is 10%.

3.4.4 Applicability of Single-Film Sh Correlations to Multiple Films and Different Air Properties

The correlations presented in the previous section were built using the single-film simulation results. The applicability of these correlations to multiple-film scenarios is important for simplified PEMFC performance models to account for realistic conditions. For the analysis of this applicability, typical multiple-film scenarios will be presented initially, followed by the characterization of single-film correlations for their applicability to multiple-film scenarios.

Multiple-film Sh results can resemble those of single-films as Δx_f becomes large enough or the set of Pe - W_f^* values becomes small enough. In multiple-film simulations, Δx_f^* took values of 1.96, 3.92, and 9.80 (corresponding to dimensional values of $\Delta x_f = 1.00, 2.00$, and 5.00 mm).

Single-film Sh correlations were characterized for their applicability to multiple-film predictions. Fig. 7 presents the local ratio of Sh_{cor} to Sh. This ratio represents the prediction accuracy and was plotted for 3 consecutive films. The plot includes 21 conditions as a result of different permutations of Pe and W_f^* as shown in Table 4. The results indicate that the largest error values can be seen in the beginning of a film and at the film wake. However, all error values are within 20%.

All multiple-film simulation results were used to characterize the accuracy of the correlations built with single-film results. Similar results were obtained to those shown in Fig. 7. These results were first transformed into absolute error percentage values ($100 \times |1 - Sh_{cor}/Sh|$) and then averaged through the flow direction for all multiple-film simulations. The resulting value is called mean absolute percentage error (MAPE) as formally defined in Eq. (38). Each down the channel location is referred to with the variable, x_t in the discrete numerical solution. For an entire number of data points, k ; the data is averaged.

$$MAPE = 100 \frac{1}{k} \sum_{t=1}^k \left| \frac{Sh_{cor}(x_t) - Sh_{num}(x_t)}{Sh_{num}(x_t)} \right| \quad (38)$$

The total number of cases is 252. These cases can be categorized into two groups based on Pe . For the range of $Pe \leq 52.32$, there are 192 cases. MAPE for these cases is 9%. Among the data points of error, 83% and 5% of

them are in between 0-10% and 10-20%, respectively. As a more challenging range of Pe , $Pe > 52.32$ covers 60 cases. In this range, MAPE is 9% as in the lower range of Pe . However, distribution of error differs by 80% and 8% of the data having an error range of 0-10% and 10-20%, respectively. Under the light of the aforementioned error characterization, the single-film based correlations can be applied to multiple-film cases with accuracy.

Although developed by using results obtained at 80 °C and 100% relative humidity, the applicability of the correlations was tested and found to be accurate down to 20 °C and 0% relative humidity. The effect of Sc on Sh at constant values of $Pe = 121.62$, $W_f^* = 0.79$, and $L_f^* = 9.82$ was numerically simulated. Since the effect of Δx_f can be neglected based on the results above, the effect of Sc was tested for a single film that results strong flow disruptions. Values of Sc for fully humidified air at temperatures of 20 and 80 °C are 0.753 and 0.632, respectively. Sc increases negligibly at temperatures lower than 20 °C since there is already a 2% increase from 40 to 20 °C. Hence, the lowest temperature to test the applicability of the correlations was selected to be 20 °C. Comparison of local Sh at 20 and 80 °C resulted in a maximum discrepancy of 3%. Variation of relative humidity from 0 to 100% has a negligible effect on Sc . The mixture of fully humidified air at 20 °C has a vapor molar fraction of 0.02. The subtraction of this marginal component to obtain dry air does not lead to a significant difference in Sc . Therefore, the reported simulation result for the effect of Sc is also applicable to dry air at 20 °C.

3.4.5 Application Example for the Sh Correlations

The correlations of Sh_{eff} provided in this study can be applied to air channels with a characterized film distribution and air velocity. This section utilizes an image from an ex-situ visualization setup that was described in detail by Banerjee and Kandlikar [10]. This setup creates the two-phase flow conditions in a flow field with parallel channels by injecting liquid water through a GDL and into channels. Fig. 8a shows a film with zero length and 0.40 mm width. This image was taken at 0.4 A cm⁻² current density, 23 °C and 0% relative humidity. These conditions correspond to a Pe of 48.

Fig. 8b shows Sh_{eff} profiles that were obtained for the visualized film through a numerical simulation and correlations. The length that the film covers in the flow direction is shown on the x axis. Since the films have zero length, the flow conditions are the most difficult to predict on the side of the films. On regions that are not covered by the film, the error percentages are below 10%. This presented approach can be applied to simplified PEMFC performance models to predict the performance loss more accurately.

3.4.6 Estimation of the Effect of the Sh Variations on Cell Performance

Variations of Sh_{eff} in air channel due to the presence of films lead to changes in local performance in a fuel cell. The change in performance can be expressed with a change in voltage for a given i . An estimation of the voltage change is made by first calculating the O_2 concentration at the GDL-air channel interface (C_{int}) with films. For this calculation, the outlet of the air channel is chosen as the reduced O_2 concentration in this region intensifies the effect of films on transport losses. Use of Sh_{eff} provides the loss of O_2 concentration from the channel mean value (C_m) to C_{int} . An additional reduction is applied to find the concentration at the cathode catalyst layer (CL), C_{CL} . The O_2 concentration loss from C_{int} to C_{CL} is due to the transport resistance of the GDL. For a dry GDL, the O_2 diffusivity can be assumed to be $D_{O_2-GDL} = D_{O_2-air}/1.5$ [32]. Lastly, the effect of changes in C_{CL} on the cell voltage (V) for a given i was calculated. The change in cell voltage from condition 1 to 2 (ΔV_{1-2}) can be expressed with the following equation:

$$\Delta V_{1-2} = \frac{R_u T}{F_c} \ln \left[\frac{C_2}{C_1} \right] \quad (34)$$

As a baseline reference, the value of $Sh_{FD,ch} = 3.349$ causes a voltage loss of 9.0 mV at $i = 1.5 \text{ A cm}^{-2}$ relative to the condition of no interfacial transport resistance ($C_{int} \rightarrow C_m$). A film with the configuration of $W_f^* = 0.98$ ($W_f = 0.50 \text{ mm}$) and $L_f^* = 9.80$ ($L_f = 5.00 \text{ mm}$) was selected along with the superficial air velocity corresponding to $Pe = 69.75$. The resulting critical points in the flow direction are $Sh_{max} = 2.19 \times Sh_{FD,f} = 2.19 \times 2.32 = 5.08$, $Sh_{ext} = 1.11 \times Sh_{FD,f} = 1.11 \times 2.32 = 2.58$, $Sh_{min} = 0.40 \times Sh_{FD,ch} = 0.40 \times 3.35 = 1.34$. Effective Sh is calculated as: $Sh_{max,eff} = Sh_{max} \times 0.61 = 3.10$ and $Sh_{ext,eff} = Sh_{ext} \times 0.61 = 1.57$. At the aforementioned i , the additional voltage drops at the positions x_{max} , x_{ext} , and x_{min} are 1, 15, and 22 mV, respectively. These values show that there is a significant voltage drop within the 5.00 mm long film. Moreover, the voltage drop at the immediate wake of the film lasts approximately 8.31 mm. Hence, the effect of the voltage drop 22 mV lasts more than the film length itself.

A comparison can be made between the impact of interfacial blockage by films and variations of Sh on the side of films. In a scenario of $W_f = 0.50 \text{ mm}$ and $i = 1.5 \text{ A cm}^{-2}$, which is the largest film width in this study, the available interfacial width is $0.61 W_{ch}$. A sufficiently long film has a $Sh_{FD,f}$ of 2.32 which is equivalent to $0.69 Sh_{FD,ch}$. If Sh is assumed to be $Sh_{FD,ch}$ on the side of a film and only the interfacial blockage is considered, Sh_{eff} of $0.61 Sh_{ch,FD}$ leads to a voltage drop 8 mV. If the interfacial blockage is neglected and only the variation of Sh is considered, Sh_{eff} of $0.69 Sh_{FD,ch}$ leads to a voltage drop of 5 mV. Due to the logarithmic dependence of

voltage loss on the transport resistance, the combination of the aforementioned resistances is significantly detrimental. A Sh_{eff} of $0.61Sh_{FD,f} = 0.61 \times 0.69Sh_{FD,ch} = 0.42Sh_{FD,ch}$ leads to a voltage loss of 20 mV.

4. Conclusions

This study numerically investigated the O_2 transport resistance at the GDL-air channel interface in PEM fuel cells. The resistance is expressed in terms of Sherwood number (Sh). The particular focus of this work was to characterize Sh under film flow conditions which are the most prevalent in an air channel. The effect of single and multiple films on Sh was expressed through correlations that are dependent on non-dimensional film width, length, and spacing, and Péclet number. These correlations can be used in simplified PEMFC performance models to better predict O_2 transport losses. Based on the results of this study, the following conclusions can be made:

- There are two fully developed Sh values: one in the channel with the absence of films ($Sh_{FD,ch}$) and another on the side of a film that is sufficiently long ($Sh_{FD,f}$). $Sh_{FD,ch}$ remains constant at 3.35. However, $Sh_{FD,f}$ varies between 2.32-2.71 with the film width.
- Films reduce the area of GDL-air channel interface for O_2 transport. This reduction has been accounted for by introducing the effective Sh (Sh_{eff}). It is equivalent to local Sh value that is reduced proportionally to the interfacial water coverage.
- In the immediate wake of a film, there is a minimum observed in Sh (Sh_{min}) which can be as low as $0.39Sh_{FD,ch}$.
- In the wake of Sh_{min} , there is a convergence trend of Sh from Sh_{min} to $Sh_{FD,ch}$. This convergence extends over a length similar to the film length. The maximum length was 13.48 mm.
- It was found that Sh on the side of a film varies significantly throughout the film length. The maximum Sh (Sh_{max}) is found at the entrance of the film and can be as high as $2.25Sh_{FD,f}$. If the film is long enough for a given Pe, Sh at the exit is $Sh_{FD,f}$.
- Correlations were developed to predict the local Sh profile for the side of a film and its wake. These correlations can be applied multiple-films. The correlations were tested against 252 multiple-film configurations. Mean absolute percentage error for Sh prediction was 9%.
- The maximum interfacial channel width blockage (39%) and Sh reduction on the side of a film (31%) lead to a voltage loss of 8 and 5 mV, respectively at a current density of 1.5 A cm^{-2} . The combined transport resistance due to the aforementioned components is a voltage reduction of 20 mV. Hence, Sh

number correlations in this study should be incorporated into simplified PEMFC models along with interfacial blockage by films.

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Table1

i [A cm ⁻²]	0.10	0.20	0.30	0.40	0.50	0.70	0.80	1.00	1.20	1.50
u_m [m s ⁻¹]	1.59	2.12	3.18	4.24	5.30	7.41	8.48	10.59	12.72	15.89
Pe	26.16	34.88	52.32	69.75	87.19	121.91	139.51	174.22	209.06	261.42

Table2

W_f [mm]	$F_{ad,GDL}$	$F_{ad,side}$	$F_{ad,top}$	F_{ad}
0.20	6.83	8.76	3.18	18.78
0.25	8.55	8.47	3.97	20.99
0.30	10.26	8.17	4.77	23.20
0.35	11.98	7.87	5.56	25.41
0.40	13.69	7.57	6.36	27.63
0.45	15.40	7.27	7.15	29.83
0.50	17.12	6.98	7.94	32.04

Table3

W_f [mm]	u_m [m s ⁻¹]							
	1.59	2.12	3.18	4.24	5.30	7.41	8.48	10.59
0.20	0.37	0.70	1.23	1.42	2.57	3.21	5.25	5.49
0.25	0.72	1.06	1.88	2.86	4.00	6.73	8.31	11.90
0.30	1.04	1.55	2.76	4.23	5.94	10.07	12.48	17.97
0.35	1.48	2.21	3.96	6.10	8.61	14.68	18.22	26.35
0.40	2.08	3.11	5.62	8.68	12.29	21.07	26.20	38.00
0.45	2.93	4.39	7.96	12.33	17.50	30.10	37.49	
0.50	4.16	6.23	11.35	17.62	25.06	43.21		

Table4

W_f [mm]	u_m [mm]						
	1.59	2.12	3.18	4.24	7.41	10.59	15.89
0.20	x	x	x	x	x	x	
0.30	x	x	x	x	x	x	
0.40	x	x	x	x	x		
0.50	x	x	x	x			

Table5

W_i^*	Pe				
	26.16	69.75	121.91	174.22	261.42
0.39	0.78	0.82	0.85	0.88	0.92
0.59	0.64	0.68	0.73	0.76	
0.78	0.53	0.58	0.63		
0.98	0.46	0.51			

Table6

W_f^*	Pe				
	26.16	69.75	121.91	174.22	261.42
0.39	1.51	2.81	3.94	4.59	3.67
0.59	1.99	4.47	4.80	1.13	
0.78	2.48	5.33	1.51		
0.98	2.81	5.14			

Table7

W_f^*	0.39	0.59	0.78	0.98
$Sh_{FD,f}$	2.71	2.47	2.33	2.32

Table8

W_f^*	Pe				
	26.16	69.75	121.91	174.22	261.42
0.39	1.25	1.38	1.47	1.55	1.65
0.59	1.43	1.66	1.85	2.00	
0.78	1.58	1.95	2.25		
0.98	1.71	2.19			

Table9

W_f^*	Pe				
	26.16	69.75	121.91	174.22	261.42
0.39	1.05	1.13	1.18	1.23	1.29
0.59	1.09	1.21	1.32	1.41	
0.78	1.13	1.32	1.49		
0.98	1.18	1.41			

Figure 1

Figure 2

b)

Figure3

a) Figure 4

b)

Figure 5

Figure 6

Figure7

Figure 8