Numerical Simulation of the Interfacial Oxygen Transport Resistance for a PEMFC Cathode Incorporating Water Droplet Coverage

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The transport resistance of oxygen in a PEMFC flow field and gas diffusion layer interface was numerically investigated in a 3D model. This model solved for the convection of air and the diffusion of oxygen in the air in a single flow field channel. The interfacial oxygen transport resistance was expressed with the Sherwood number. For a dry channel, the numerically obtained Sherwood number was validated by the relationship between Nusselt and Sherwood numbers through the Lewis number. Following the validation, the model simulated conditions of a single water droplet that remained adhered on the flow field and gas diffusion layer interface. The effects of droplet size, flow velocity, and variations in vapor content in air due to changes in temperature were analyzed and discussed. For the selected range of droplet sizes and flow velocities, numerically obtained drag forces were compared against experimentally obtained adhesion forces.

Introduction

Proton exchange membrane fuel cells (PEMFCs) are electrochemical engines which transform the chemical energy in hydrogen into electrical energy. They are strong candidates to be the successor of internal combustion engines. Their environmentally friendly by-products provide them an important advantage against internal combustion engines. PEMFCs dissipate heat and produce water as their by-products. However, the liquid water produced in the PEMFC can partially block the pores of gas diffusion layer (GDL) and thereby hinder the reactant diffusion. Moreover, the heat generated needs to be removed without overcooling the system to avoid excess condensation of water vapor, which leads to the blockage of GDL pores. The management of these by-products is an active area of research to enhance the fuel cell performance as much as possible.

PEMFCs produce high power output at high current and low voltage operation points. At these conditions and at a given current, the major source of voltage drop is the transport losses of oxygen on the cathode side. As the oxygen concentration at the catalyst layer decreases, the voltage of the cell decreases drastically. Due to this source of voltage drop, it is important for researchers to accurately model the concentration drop from the cathode flow field (FF) to the catalyst layer (CL). Down-the-channel performance model by Gu et al. is a pseudo-2D numerical model which incorporates a wide range of operation parameters but still treats them with simplifications so the model can be applied to large scale and solved conveniently (1). This performance model
numerically simulates the through-plane transport in a fuel cell which is also discretized in the down the flow field direction. The pseudo-2D nature of this model comes from the fact that down the channel discretized fuel cell sections can only communicate in-plane through the flow fields which represent parameters such as reactant concentration and pressure, and coolant temperature. This model incorporates the oxygen concentration drop at the GDL-FF interface. This drop is comparable to the one in the GDL and cannot be neglected. For the better modeling of fuel cells, current distributions along the channel bear importance. An example case was presented by Ju and Wang showing that it was possible to obtain the same average current density from two numerical fuel cell models with different distributions of local current densities (2). Hence, it is important to accurately characterize the oxygen resistance at the GDL-FF interface as a function of down the FF channel length.

For a given fluid flow and species diffusion problem in a flow channel, the concentration drop at the interface is characterized by the mass transfer coefficient \( h_m \). This parameter is non-dimensionalized and becomes the Sherwood number (Sh), which is the mass transfer equivalent of Nusselt number (Nu) for heat transfer problems. For a fluid flow in a specific geometry and a specific boundary condition, Nu can be linked to Sh through the use of Lewis number (Le). For a wide range of rectangular channel aspect ratios, and uniform heat flux at a single channel wall, Nusselt number values are provided in the available literature (3). These values can be mapped through \( \text{Sh} = \text{Le}^{1/3} \text{Nu} \) (4). Therefore, the interfacial oxygen resistance at a dry cathode FF can be predicted by the already established Nu knowledge for a variety of channel geometries and boundary conditions.

In the practical case of a fuel cell, the diffusion resistance at the GDL-FF interface is not constant throughout the channel length. The liquid water introduced into the channel through the GDL pores blocks a significant portion of the GDL-FF interface. The liquid water from the pores first takes form of droplets. As the droplets proceed towards the channel outlet, they first coalesce into films and then into slugs (5). Therefore, the water coverage ratio, defined as the area covered by water on the GDL-FF interface, gradually increases from the channel inlet to outlet as more water is introduced into channels. The gas flow in the channels is responsible for the propagation of liquid features towards the channel outlet under negligible gravitational forces. Gopalan and Kandlikar studied the tendency of droplets to fill into the corners of GDL and FF side walls under the effect of air flow (6). The corner filling condition leads droplets to form larger water features such as films or slugs, and also increases the drag force to break their adhesion at the GDL-FF corner compared to a stand-alone droplet on the GDL. Das et al. took an isolative approach to water droplets and experimentally obtained their adhesion forces with the utilization of gravitational force acting on the droplets on an inclined GDL surface (7). Turhan et al. utilized neutron imaging of a fuel cell to show that with the decreased gas flow rates more liquid water occupied FF channels and covered the GDL-FF interface (8). This water coverage was reported via transparent fuel cells in the visible spectrum for the entire GDL-FF interface (5, 9). It was also experimentally proven that the spatio-temporal distributions of local cell current density and water slugs at the GDL-FF interface demonstrate a parallelism (10).

Studies on Sh in PEMFCs are scarce in the available literature. All the studies reported here from the available literature approached the problem by treating FF
channels as two parallel walls. In these works, the characteristic lengths to non-dimensionalize the mass transfer coefficient were selected differently and this led to different Sherwood number values. This also introduced inconsistencies in the heat-mass transfer analogy as the hydraulic diameter is often used in reporting Nu. For comparison purposes, Sh values will be reported here with the characteristic length of hydraulic diameter. Sherwood numbers were also compared against theoretical predictions which differed based on the operating conditions. In their numerical model, Wang et al. obtained Sh of 5.274 while the theoretical prediction was 5.386 (11). In 2007, Jeng et al. simulated the cathode side of a 2D fuel cell with a FF consisting of two parallel plates (12). They simulated air flow velocities corresponding to a maximum fuel cell current density of 0.5 A/cm² along with a stoichiometry of 2. All flow velocities led to a fully developed Sh of 6 which was within 2.66% with the analytical prediction based on Sh-Nu correlation. Hassanzadeh et al. numerically simulated an entire 2D fuel cell which yielded Sh for the cathode air flow: 5.411 (13). The aforementioned studies are limited with their 2D FF assumption. In a 3D FF, the side walls have a considerable effect on the velocity profile developed in the channel. The 2D and 3D Sherwood numbers can lead to the same hₘ for a certain channel cross section. However, this assumption cannot be applied for channels with different aspect ratios. Moreover, all these works were based on another assumption that FF channels were not occupied by liquid water features. Liquid water can be transported into the FF through the GDL and take the form of droplets, films or slugs. As a result, a portion of the GDL-FF interface is blocked and the flow velocity profile in the FF is disrupted around the water features. It is important to investigate how the interfacial oxygen resistance is affected by the presence of water in FFs.

This work aims to provide the Sherwood number specifically for 3D FF geometries while incorporating the presence of liquid water. Droplets were chosen as the liquid features to be investigated due to the fact that they lead to more complex features such as films or slugs. In a FF channel with a hydraulic diameter of 0.51 mm, the air convection and the diffusion of oxygen were numerically simulated by a commercial software package, COMSOL Multiphysics® 4.3. The droplet presence was mimicked in the channel by introducing a droplet-shaped obstruction. The effects of the droplet size, air velocity, and variations in vapor content in air due to changes in temperature were investigated. The results are presented as local and down-the-channel-averaged Sh. Down the channel averaged Sh was calculated only on the portions of the channel where the droplet altered the fully developed Sh values. In order to report the adhesion possibility of each droplet size under the air flow, the net drag on different droplet sizes was numerically calculated and compared against reported droplet adhesion forces which had been obtained experimentally.

Methodology

Introduction to the Problem Geometry and Physics

In this numerical study, the selected FF design meets the transportation targets of the United States Department of Energy (14). Figure 1 depicts a repeating portion of this design. Among the parallel FF channels, a single channel alone was simulated to investigate the Sh. The channels were 183 mm long but only 60 mm was simulated. The full channel length of the design was used only to calculate the air flow velocities. The channel width and height were $W \times H = 0.7$ mm $\times$ 0.4 mm respectively, and they led to a
hydraulic diameter of \( d_h = 0.51 \text{ mm} \). The aspect ratio of the channel cross section was defined as \( \alpha = H/W = 0.57 \). The land regions between each channel were 0.5 mm wide (channel side to symmetry plane: 0.25 mm) which also contributed to air flow velocity calculations.

The effect of a droplet in the FF was mimicked by placing a representative droplet shaped obstruction in the numerical domain, 30 mm away from the inlet \((x_d = 30 \text{ mm})\). Hence, the simulation of air convection was strictly single-phase. The height of the FF channel constrained the droplets to be shorter than 0.4 mm. By calculating the Bond number, the relative contribution of gravity to the droplet shape was evaluated. The resulting Bond number: 0.053 showed that the largest possible droplet shape would be dominated by the surface tension. By exploiting this fact, as shown in Fig. 2, the droplet shape was assumed to be a sphere which was partially cut to be placed at the GDL-FF interface \((z = 0)\) with a contact angle of \( \theta = 147^\circ \). This hydrophobic contact angle was chosen to represent common static contact angle measurements in the available literature \((6, 7)\). The droplet size was characterized with the radius of the sphere representing it, \( r \). The cut portion of the droplet, \( b \) was calculated to comply with the contact angle. At a given \( y-z \) cross section, the total channel width, \( W \) at the GDL-FF interface could be blocked by the droplet for a wet interface width, \( W_{\text{wet}}(x) \). This directly affected the dry GDL-FF interface width that can be utilized for oxygen diffusion. Moreover, by using the wetted perimeter of the droplet footprint, \( P \) the droplet adhesion force can be calculated based on experimental correlations by Das et al. \((7)\). By numerically obtaining the net drag on the droplet in the flow direction \( F_D \), and comparing it to the adhesion force, \( F_{\text{Ad}} \) the possibility of encountering that specific droplet size and therefore, the Sh can be predicted. Table I provides \( r, P \), and the net droplet height \((H_d)\).

Figure 1. The cross sectional geometry of the FF and GDL.

Figure 2. The \( y-z \) cross sectional geometry of a droplet in the FF channel.
The air flow velocity in the FF channel was calculated based on the molar consumption rate of oxygen, and stoichiometry. The calculations were based on the operating conditions of 1 atmosphere pressure \((p)\), 80 °C temperature \((T)\), and 100% relative humidity \((RH)\). Table II presents the equivalent molar fluxes at the GDL-FF interface \(\left(j_{\text{GDL-FF}}\right)\) and mean air velocities \((u_m)\) for a current density \((i)\) range from 0.1 to 1.5 A/cm\(^2\) and the corresponding stoichiometry ratios \((\lambda)\). The mean air velocity was assumed to be constant throughout the channel.

The diffusivity of oxygen in the air \((D_{O_2-air})\) was estimated to be 0.31 cm\(^2\)/s by Wilke’s formula which took molar fraction based averages of oxygen diffusivity in nitrogen and water vapor (15). The molar fraction of vapor was first calculated through the vapor saturation pressure correlation (16). The remaining dry air fraction was assumed to have a 21/79 distribution of oxygen and nitrogen. The molar fractions were fed into Wilke’s formula along with the component diffusivities (oxygen-nitrogen and oxygen-water vapor) obtained with the correlation by Fuller, Schettler and Giddings (17).

The presence of vapor also affected the material properties related to equations of air momentum conservation. The density, \(\rho\) and dynamic viscosity, \(\mu\) of air were calculated as 0.828 kg/m\(^3\) and 1.625×10\(^{-5}\) Pa∙s, respectively due to correlations which provided these parameters under the condition of RH = 100% as a function of temperature (18).

**Definitions of the Interfacial Oxygen Resistance**

In a FF channel as shown in Fig. 2, the mass transfer coefficient, \(h_m(x, y)\) relates the molar flux of oxygen at the GDL-FF interface \((j\text{ at } z = 0 \rightarrow j_{\text{GDL-FF}})\) to the concentration drop at the same interface. The concentration drop at the interface is the difference between the bulk fluid concentration of oxygen, \(C_\infty\) and local oxygen concentration at a given point on the GDL-FF interface, \(C(x, y, z = 0)\). The problem was assumed to be governed by Fick’s diffusion equation. Therefore, \(j_{\text{GDL-FF}}\) can be expressed by Fick’s diffusion equation:

\[
h_m(x, y) = \frac{j_{\text{GDL-FF}}}{[C_\infty - C(x,y,z=0)]} = - \frac{D_{O_2-air}}{[C_\infty - C(x,y,z=0)]} \frac{\delta C}{\delta z}|_{z=0}
\]
can be defined only on the dry GDL-FF interface as there is no concentration gradient on the wet GDL-FF interface. In order to enable \( h_m \) to be defined everywhere at the GDL-FF interface, it was transformed into a piecewise function which output zero at the wet GDL-FF interface. This function is called the effective mass transfer coefficient, \( h_{m,\text{eff}} \):

\[
h_{m,\text{eff}} = \begin{cases} 
\text{Dry surfaces:} & h_m \\
\text{Wet surfaces:} & 0 
\end{cases}
\]  

[2]

Variations of \( h_{m,\text{eff}}(x, y) \) along the channel width were averaged into the channel-width-averaged effective mass transfer coefficient, \( \overline{h_{m,\text{eff}}}(x) \):

\[
\overline{h_{m,\text{eff}}}(x) = \frac{1}{W} \int_{y=0}^{W} h_{m,\text{eff}} \, dy
\]  

[3]

In order to understand the mass transfer characteristics only on the dry GDL-FF interface, the effect of water coverage was removed by scaling \( \overline{h_{m,\text{eff}}}(x) \) with the ratio between channel and dry interface width. The resulting dry-region-averaged mass transfer coefficient, \( \overline{h_m}(x) \) only represents the mass transfer on the dry GDL-FF interface.

\[
\overline{h_m}(x) = \overline{h_{m,\text{eff}}}(x) \frac{W}{(W-W_{\text{wet}})}
\]  

[4]

The Sherwood number is the non-dimensionalized expression of the mass transfer coefficient. By non-dimensionalizing \( \overline{h_m}(x) \) with the hydraulic diameter, \( d_h \) and the diffusivity of oxygen in air, \( D_{O_2-\text{air}} \) the dry-region-averaged Sherwood number was obtained, \( \text{Sh} \):

\[
\text{Sh} = \frac{\overline{h_m}}{D_{O_2-\text{air}}} \frac{d_h}{D_{O_2-\text{air}}}
\]  

[5]

The fully developed Sherwood number (\( \text{Sh}_{FD} \)) for a dry channel can be expressed with its heat transfer equivalent, fully developed Nusselt number, \( \text{Nu}_{FD} \). These two non-dimensional numbers are related to each other through the non-dimensional Lewis number (\( \text{Le} \)) (4):

\[
\text{Sh}_{FD} = \text{Nu}_{FD}(\text{Le})^{1/3} = \text{Nu}_{FD} \left( \frac{k}{\rho C_p D_{O_2-\text{air}}} \right)^{1/3}
\]  

[6]

Lewis number uses the thermal conductivity (\( k \)) and heat capacity (\( C_p \)) of air in addition to \( \rho \) and \( D_{O_2-\text{air}} \). \( k \) and \( C_p \) were calculated as 0.0266 W/(m.K) and 1349.9 J/(kg.K), respectively for air under the aforementioned operating conditions (18). With the calculated input parameters, the mapping coefficient \( \text{Le}^{1/3} \) was obtained to be 0.915. This coefficient was applied to the \( \text{Nu}_{FD} \) obtained from a numerical study which simulated single-phase convection in rectangular channels under constant circumferential and axial heat flux boundary condition, also known as H2 boundary condition (3). This work reported a \( \text{Nu}_{FD} \) of 3.584 for the channel aspect ratio, \( \alpha = 0.57 \) and only one of the
long sides under constant heat flux (H2). The mapping of this \( \text{Nu}_{FD} \) with Lewis number resulted a \( \text{Sh}_{FD} \) of 3.279.

The dry-region-averaged Sherwood number was expected to diverge from \( \text{Sh}_{FD} \) at the upstream and downstream vicinity of the droplet. Down the channel effects of the droplet was quantified by averaging \( \text{Sh} \) values where they diverged from \( \text{Sh}_{FD} \). This parameter was called dry-region-and-down-the-channel-averaged Sherwood number, \( \text{Sh}_{av} \). The point where \( \text{Sh} \) started to diverge from \( \text{Sh}_{FD} \) at the droplet upstream was spatially referred as \( x_{dL} \) where \( L_u \) was the length of the region affected at the upstream of the droplet. Similarly, the end of the droplet wake region was spatially referred as \( x_{dL_d} \) where \( L_d \) was the length of the wake region. By using these parameters, \( \text{Sh}_{av} \) can be defined as:

\[
\text{Sh}_{av} = \frac{1}{L_u+L_d} \int_{x=x_d-L_u}^{x_d+L_d} \text{Sh}(x) \, dx
\]  

\[7\]

**Numerical Implementation**

The physical problem described above was numerically simulated as a 3D model and solved by a commercially available software package, COMSOL Multiphysics®. This model consisted of an isolated FF channel domain from which a droplet shaped obstruction was removed. Figure 3 shows the remaining domain represented only the volume that air flowed. The channel had a length of \( L=60 \text{ mm} \). The droplet was placed 30 mm away from the inlet and centered in the channel width, \( W \).

![Figure 3. The simulated numerical domain representing a FF channel with a droplet shaped obstruction introduced inside.](image)

In this domain, stationary incompressible Navier-Stokes equations and Fick’s diffusion equation were solved along with their respective continuity equations. It was assumed that air properties remained the same under oxygen consumption. By exploiting this assumption, Navier-Stokes equations along with continuity were solved first for the velocity vector, \( \textbf{u} \):

\[
\rho (\textbf{u} \cdot \nabla) \textbf{u} = \nabla \cdot \left[-\rho \mathbf{I} + \mu (\nabla \textbf{u} + (\nabla \textbf{u})^T)\right]
\]

\[8\]

\[
\rho \nabla \cdot \textbf{u} = 0
\]

\[9\]

Following the solution of Eqs. 7 and 8, the oxygen flux vector, \( \textbf{j} \) was calculated due to the diffusive term governed by Fick’s diffusion equation, and the convective term
provided by the formerly solved velocity vector, \( u \). The continuity of species was solved with the conservative formulation:

\[
\begin{align*}
      j &= -D_{O_{2}-\text{air}} \nabla C + uC \quad [10] \\
      \nabla \cdot (-D_{O_{2}-\text{air}} \nabla C + uC) &= 0 \quad [11]
\end{align*}
\]

At the inlet, a uniform flow velocity was set to be \( u_m \) in the \( x \) direction, and a uniform oxygen concentration, 3.836 mol/m\(^3\). At the outlet, the pressure was set to be zero and the oxygen flux normal to this boundary was only due to air convection. At the bottom surface of the channel which represents the GDL-FF interface, the diffusive molar flux of the oxygen, \( j \) in the surface normal direction (\( z \)) was set to be \( j_{GDL-FF} \). The footprint of the droplet did not contribute to the oxygen flux. On every channel side wall and droplet surface no-slip boundary condition was imposed.

In order to reduce the complexity of the numerical problem, the domain was divided into five sub-domains which were serially connected in the flow direction. By sequentially solving these sub-domains in the flow direction, the full solution was obtained. During this process, it was observed that a droplet can affect the solution up to 1 mm upstream. The droplet was therefore positioned 2 mm away from the inlet of its respective sub-domain.

The oxygen concentration (\( C \)), air velocity vector (\( u \)) and pressure field (\( p \)) were discretized with third, third and second order elements, respectively. The maximum mesh element size used was 0.08 mm. Each subdomain had 90,000 to 120,000 tetrahedral elements. The corresponding number of degrees of freedom for each subdomain was approximately \( 2 \times 10^6 \). The problem was solved by Generalized Minimal Residual Method (GMRES) with the utilization of geometric multigrid. All variables were required to converge to a tolerance of \( 10^{-6} \).

Results

Effects of Flow Velocity and Droplet Size on the Dry-Region-Averaged Sherwood Number

The GDL-FF interface was subject to a range of air velocities \( u_m = 1.59 \) – 15.89 m/s which correspond to a current density range of 0.1 – 1.5 A/cm\(^2\) under the given operating conditions provided in Table II. The average oxygen transport resistance at a dry FF-GDL interface that is located at a given \( y-z \) cross section was characterized by the dry-region-averaged Sherwood number, Sh. Dry-region-averaged Sherwood number demonstrates variations of the oxygen transport resistance only in the flow direction. Each flow velocity was expected to converge to the same fully developed Sherwood number, \( \text{Sh}_{FD} \). Figure 4 shows the Sh profile for the first 28 mm length of the channel which was subject to three different \( u_m \). For \( u_m \) values of 1.59, 4.24 and 15.89 m/s, the respective developing lengths, \( L_{dev} \) were 3.34, 8.02 and 23.11 mm. All flow conditions converged to a \( \text{Sh}_{FD} \) of 3.36 for locations \( x \geq L_{dev} \). By using the Nu-Sh analogy, the theoretical value of a fully developed Sh is calculated to be 3.279 for a channel with one wall under constant mass flux and three other impermeable walls (3). A 2.5% deviation shows that there is a good agreement between the theoretical and numerical \( \text{Sh}_{FD} \).
Figure 4. The effect of the inlet velocity, $u_m$, on the developing length of the dry-region-averaged Sherwood number, $Sh$.

Figure 5 shows the results for a droplet positioned 30 mm away from the inlet. Under varying $u_m$, down the channel variations in $Sh$ were analyzed for a droplet size of $r = 0.15$ mm. While $u_m$ was 1.59 m/s, $Sh$ started to decrease at the upstream of the droplet, reached the minimum on the droplet, and recovered back to the $Sh_{FD}$ value at the droplet downstream. Both $u_m = 4.24$ and 15.89 m/s showed a minimum $Sh$ on the droplet as well. However, they were differentiated from the lowest $u_m$ by leading to an increase in $Sh$ at the droplet upstream. The highest $u_m$ was differentiated from the other two at the near downstream. The maximum $Sh$ in this region was 40% larger than $Sh_{FD}$. The two other two flow velocities could not result this much of a $Sh$ increase. The wake region for the highest $u_m$ was 24 mm.

There can be two conclusions drawn from Fig. 5. Firstly, at low flow velocities, the droplet can decrease the $Sh$ around it because of the altered hydrodynamic conditions adverse to oxygen mixing on the GDL-FF interface. Hence, the interfacial oxygen resistance increases not only due to water coverage but also altered hydrodynamic conditions. Secondly, at high flow velocities, droplets act as ideal flow disrupters. They
can change hydrodynamic conditions in favor of oxygen mixing at the droplet downstream. Since droplets are short in the direction of flow, mixing effects at the downstream are not overshadowed by the water coverage as it could happen under film conditions. The transition from decreased to increased $Sh$ at the droplet downstream is dependent on the flow velocity.

Figure 6 presents the effect of droplet size on $Sh$ at the highest flow velocity, $u_m = 15.89$ m/s. All droplet sizes led to a sharp peak of $Sh$ at the droplet upstream, and a minimum $Sh$ on the droplet. The smallest droplet size ($r = 0.10$ mm) led to an almost negligible increase in $Sh$ at the downstream with a maximum change of 3% over $Sh_{FD}$. The largest two droplets ($r = 0.15$ and 0.20 mm) resulted significant increases in $Sh$ with the respective maximum changes over $Sh_{FD}$: 40% and 82%. In the vicinity of all three droplets, it was observed that there was no $Sh$ smaller than $Sh_{FD}$. This shows that if a certain threshold value of $u_m$ is exceeded, droplets can only increase the $Sh$ around them. Another observation is on the wake regions of $r = 0.15$ and 0.20 mm: Although the larger droplet led to larger peak of $Sh$, the wake regions of both droplet sizes converged to the same line around $x = 38$ mm before they reached to $Sh_{FD}$. This can mean that a second droplet placed further than $x = 38$ mm could lead to the same $Sh$ profile at the downstream of itself because both sizes for the first droplet would leave the same mixing effects as a heritage to the second droplet. However, this would differ if the second droplet was placed closer to the first one than $x = 38$ mm.

![Figure 6. The effect of the droplet size, $r$ on the variations of the dry-region-averaged Sherwood number, $Sh$: $u_m = 15.89$ m/s.](image)

**Comparison between Air Drag on a Droplet and Droplet Adhesion Force**

The upper limit of simulated droplet sizes was defined by the geometrical properties of the FF. After performing the simulations, a new criterion could be utilized to predict the possibility of observing $Sh$ trends as reported above. A way of predicting this possibility was to compare numerically obtained drag forces on droplets in the flow direction, $F_D$ against experimentally obtained adhesion forces due to the surface tension, $F_{Ad}$. The adhesion force of an ideally shaped droplet was reported per wetted perimeter, $P$ (7). For aged SGL 24BA and 24DA GDLs, the adhesion forces per wetted perimeter were 22 and 17 $\mu$N/mm, respectively (7). As a mid-value 20 $\mu$m/mm was selected. The aged
state of the GDL offers a better adhesion and it reflects long-term operating conditions of a fuel cell. The adhesion force of a droplet at a particular size was found by \( F_{Ad} = 20 \mu m/mm \times P \) where \( P \) was reported in Table I. Table III shows a comparison between the drag and adhesion forces. Underlined \( F_D \) values represent lower ones than \( F_{Ad} \) values.

### Table III. Drag Forces on Droplets in the Flow Direction (\( F_D \)) and Adhesion Forces (\( F_{Ad} \))

<table>
<thead>
<tr>
<th>( r ) (mm)</th>
<th>( u_m = 1.59 \text{ m/s} )</th>
<th>( u_m = 4.24 \text{ m/s} )</th>
<th>( u_m = 15.89 \text{ m/s} )</th>
<th>( F_{Ad} ) (( \mu N ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10</td>
<td>0.20</td>
<td>0.78</td>
<td>5.86</td>
<td>6.84</td>
</tr>
<tr>
<td>0.15</td>
<td>0.64</td>
<td>2.35</td>
<td>18.00</td>
<td>10.17</td>
</tr>
<tr>
<td>0.20</td>
<td>2.07</td>
<td>8.00</td>
<td>58.10</td>
<td>13.57</td>
</tr>
</tbody>
</table>

The results in Table III show that the droplet sizes \( r = 0.15 \) and \( 0.20 \) mm cannot be expected to adhere to the surface when exposed to the air flow velocity, \( u_m = 15.89 \text{ m/s} \). It can be expected to observe droplets almost as large as the FF height for \( u_m = 1.59 \) and \( 4.24 \text{ m/s} \). At the highest \( u_m \), it is not expected to have FF to be blocked by droplets as they would be sheared off before they further grow. The possibilities mentioned here also have reflections on the expected Sh trends. The largest two droplet sizes could create significant increases in Sh when they were exposed to the highest flow velocity, \( u_m = 15.89 \text{ m/s} \). However, the adhesion forces are not strong enough to keep them on the GDL-FF interface. Therefore, depending on the flow velocity, \( \text{Sh}_{av} \) around the droplet is expected to be slightly smaller or larger than \( \text{Sh}_{FD} \).

The Dry-Region-and-Down-the-Channel-Averaged Sherwood Number and the Wake Lengths of the Droplets

Down the channel variations of Sh in the vicinity of the droplet were quantified by the dry-region-and-down-the-channel-averaged Sherwood number, \( \text{Sh}_{av} \) as defined in Eq. 7. \( \text{Sh}_{av} \) becomes more meaningful if the droplet wake length, \( L_{wake} \) is known along with it. Hence, the length affected by \( \text{Sh}_{av} \) can be envisaged easier. Table IV provides \( \text{Sh}_{av} \) and \( L_{wake} \) values which are underlined if they were reported in Table III that they could adhere to the GDL-FF interface at their respective flow velocities.

### Table IV. Dry-Region-and-Down-the-Channel-Averaged Sherwood Numbers (\( \text{Sh}_{av} \)) and Length of Wake Regions (\( L_{wake} \))

<table>
<thead>
<tr>
<th>( \text{Sh}_{av} )</th>
<th>( L_{wake} ) (( \text{mm} ))</th>
<th>( u_m = 1.59 \text{ m/s} )</th>
<th>( u_m = 4.24 \text{ m/s} )</th>
<th>( u_m = 15.89 \text{ m/s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10 mm</td>
<td>3.21</td>
<td>3.28</td>
<td>3.29</td>
<td>4.21</td>
</tr>
<tr>
<td>0.15 mm</td>
<td>3.24</td>
<td>3.57</td>
<td>3.36</td>
<td>8.82</td>
</tr>
<tr>
<td>0.20 mm</td>
<td>3.27</td>
<td>3.71</td>
<td>3.36</td>
<td>7.68</td>
</tr>
</tbody>
</table>

Table IV shows that there is a consistent increase in \( L_{wake} \) with \( u_m \). Although the droplet size, \( r \) has mostly the same effect on \( L_{wake} \), its consistency is questionable due to the \( r = 0.15 \) mm to \( 0.20 \) mm transition when \( u_m = 4.24 \text{ m/s} \). The same droplet size transition at the highest \( u_m \) did not also give a clear increase in \( L_{wake} \). It is thought that the air flow started to be disrupted in a different way, as the channel approached to be fully blocked. \( L_{wake} \) became significant such that a second water feature can possibly remain in the wake length of the first droplet. For an example of \( r = 0.15 \) mm and \( u_m = 4.24 \text{ m/s} \), the wake region (also depicted in Fig. 5) can incorporate another droplet which would disrupt the flow even stronger and lead to a significant increase in Sh. It is reasonable to
expect a series of droplets leading to significantly increased \( \text{Sh}_{av} \) values. For isolated droplets, \( \text{Sh}_{av} \) values can be larger than \( \text{Sh}_{FD} \) only when \( u_m \) is at the highest. However, only the smallest droplet size can remain adhered at this flow velocity.

**The Effect of Vapor Content in the Air on the Dry-Region-Averaged Sherwood Number**

In this study, the operating temperature had an impact on the air flow velocities and oxygen diffusivities in the air. Under the given RH = 100% condition, the largest effect on the flow velocity was the added water vapor mass into the air mixture. By fully saturating the air at 20 °C and 80 °C, the flow velocity can differ 122% with the increased temperature. Figure 7 demonstrates the effect of this phenomenon on \( \text{Sh} \) for the largest droplet size, \( r = 0.20 \text{ mm} \), \( i = 1.5 \text{ A/cm}^2 \), and \( \lambda = 2 \). The corresponding velocities for 20 °C and 80 °C were 7.15 m/s and 15.89 m/s, respectively. The higher air velocity at 80 °C led to a higher \( \text{Sh} \) around the droplet and a longer wake region compared to the case at 20 °C. The change in the air velocities was not quadratically reflected on the droplet drag forces. The drag forces at 20 °C and 80 °C were 21.80 \( \mu \text{N} \) and 58.10 \( \mu \text{N} \), respectively. Due to the change of the velocity from 20 °C to 80 °C case was almost 2 times, the drag could be expected to increase around four times. However, \( F_D \) at \( T = 80 \) °C was 2.66 times the \( F_D \) at \( T = 20 \) °C. This can be explained by the increased density and viscosity of the RH=100% air with the temperature decrease. The density and viscosity became 1.19 \( \text{kg/m}^3 \) and 1.79\( \times10^{-5} \) \( \text{Pa} \cdot \text{s} \), respectively at 20 °C (18). Therefore, drag forces on droplets cannot be directly mapped in between temperatures by just referring to their respective flow velocities.

![Figure 7: The effect of the vapor content in the air due to temperature changes on the dry-region-averaged Sherwood number, \( \text{Sh} \) at the dry channel interface remaining from the water coverage: \( r = 0.20 \text{ mm} \), \( i = 1.5 \text{ A/cm}^2 \), and \( \lambda = 2 \).](image)

Another impact by the presence of the water vapor in the air was the change of oxygen diffusivity in the air. The diffusivities of oxygen in the air at 20 °C and 80 °C were 0.20 and 0.31 \( \text{cm}^2/\text{s} \), respectively. The increased diffusivity shortens the developing length and the wake region. Therefore, for the same flow velocities, lower diffusivities can lead to longer wake regions at the droplet downstream and so, larger \( \text{Sh}_{av} \) values. Moreover, the Nu-Sh correlation through \( \text{Le} \) was also affected by the changes of the air properties input to \( \text{Le} \). At 20 °C and 80 °C, the coefficients of \( \text{Le}^{1/3} \) in Eq. 6 were 1.042
and 0.915, respectively. However, the change in \( Le^{1/3} \) was not obtained in the numerically obtained \( Sh_{FD} \). The 1/3 exponent on \( Le \) and/or the simulation accuracy may lead to this divergence between the correlation based and numerically obtained \( Sh_{FD} \).

**Conclusions and Future Work**

A stationary 3D numerical model was solved to investigate the oxygen transport resistance at a fuel cell flow field and gas diffusion layer interface. The interfacial resistance of oxygen was reported in the non-dimensional dry-region-averaged Sherwood number. The results lead to the following conclusions and future work directions:

- The numerically obtained fully developed Sherwood number, 3.36 in a dry channel with an aspect ratio, 0.57 was validated by the Nusselt - Sherwood number similarity condition through the Lewis number. The presence of a water droplet on the flow field and gas diffusion layer interface was shown to affect the dry-region-averaged Sherwood number in the droplet vicinity.

- The dry-region-averaged Sherwood number around the droplet and at the dry channel interface remaining from the water coverage becomes larger than the fully developed value with the droplet size and flow velocity. The dependency of the dry-region-averaged Sherwood number on these parameters becomes stronger as the parameters approach to their upper limiting values. As these parameters approach their lower limits, dry-region-averaged Sherwood number can even be lower than the fully developed value around the droplet.

- The possibility of a droplet remaining adhered to the surface when subjected to an air flow was evaluated by comparing the numerically obtained drag force on the droplet against the droplet adhesion force provided by an experimental study in the literature. The force comparison study showed that a significant increase in the dry-region-averaged Sherwood number is not possible due to the lack of adhesion force to keep the droplet adhered while disrupting the flow.

- For the parameters in this study, the maximum practically achievable increase of the dry-region-averaged Sherwood number with respect to the fully developed value by a single droplet can be 3% within an 18 mm of droplet wake region.

- The vapor content in the air was shown to have a direct effect on the flow velocity due to increasing temperatures in fully saturated streams. For the same current density and stoichiometry, the dry-region-averaged Sherwood number can be increased significantly due to an increase in vapor content in the air.

- In air compositions at higher temperatures, the decreasing density and viscosity of the saturated air with the larger molar fraction of water vapor reduces the effect of an increased flow velocity on the droplet drag.

- A significant increase in the dry-region-averaged Sherwood number may be achieved by placing droplets in series within their wake regions. Hence, the droplets may induce more flow mixing in multiple stages without being exposed to an excessive air drag. This investigation is one of the directions of future work.

- Another future direction is the investigation of the droplet position across the channel width. The droplet can either be forced from the center width of the channel towards the channel corners, or it can originate closer to corners. A commonly observed situation is the pinning of the droplet to the corners. Due to the stronger adhesion provided at the channel corners, droplets can reside in the
channels at larger sizes and increase the dry-region-averaged Sherwood number significantly.

Acknowledgments

Support for this project was provided by the US Department of Energy under award number: DE-EE0000470.

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