EFFECT OF WATER REMOVAL THROUGH THE GAS DIFFUSION LAYER AND FLOW FIELD ON PROTON EXCHANGE MEMBRANE FUEL CELL PERFORMANCE

by

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B.A.Sc., The University of British Columbia, 2013

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

MASTER OF APPLIED SCIENCE

in

THE COLLEGE OF GRADUATE STUDIES

(Mechanical Engineering)

THE UNIVERSITY OF BRITISH COLUMBIA

(Okanagan)

October 2015

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ABSTRACT

The sustainable nature of fuel cells has attracted global attention, and major automotive companies are investing in their development. A proton exchange membrane fuel cell (PEMFC) combines hydrogen and oxygen to produce electricity, with only heat and water as by-products. The water produced in the reaction must be effectively removed to avoid flooding, whereby liquid water accumulates in the porous electrodes and blocks pathways for reactant diffusion. By impeding reactant transport, ineffective water management decreases cell performance. Hence, understanding water removal mechanisms in PEMFCs is critical in order to increase their performance and yield a viable alternative to present-day technologies.

This study investigates the effects of water removal through the gas diffusion layer (GDL) and flow field of PEMFCs in order to elucidate the impact they have on output power performance. A novel technique is implemented to evaluate the joint influence of the inlet air flow rate (FR) and relative humidity (RH), which drive water removal processes. The technique consists of an in-situ experiment that assesses cell performance, in combination with a quasi in-situ experiment that captures the local rates of water removal through the GDL along the length of the flow field. Findings from the in-situ experiment indicate a positive effect of FR, a negative effect of RH, and an interaction between FR and RH. The highest performance results from a high air FR (stoichiometric value of 6 at 1 A/cm²) and 65% RH air input, resulting in a power density of 0.470 W/cm². Based on findings from the quasi in-situ experiment, diffusivity was extracted using a comprehensive model. The final effective water vapor diffusion coefficient of the studied GDL was 0.0481 cm²/s at 70°C.

Results from the experiments were compared and the association between performance and water removal rates was analyzed. High in-situ performance is most likely to occur when the quasi
in-situ water removal rates are above an in-situ water production rate at 1 A/cm². The results from the input conditions are discussed in relation to water removal characteristics and potential flooding of the electrodes. Ultimately, this thesis provides valuable insight into water management aspects of PEMFCs.
PREFACE

The research presented in this thesis is the original work of the author. The research was conducted under the supervision of Dr. Mina Hoorfar at the Advanced Thermo-Fluidic Laboratory (ATFL) in the School of Engineering at UBC Okanagan. This research was funded, in part, by the Natural Sciences and Engineering Research Council of Canada (CGS M - 444649 – 2013). The gas diffusion layer sample used in this study was provided by, and used with the permission of, Ballard Power Systems Inc. To date, this work has not been published elsewhere, in part or in full.
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# NOMENCLATURE

## Abbreviations

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<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>CCM</td>
<td>Catalyst coated membrane</td>
</tr>
<tr>
<td>CL</td>
<td>Catalyst layer</td>
</tr>
<tr>
<td>FR</td>
<td>Flow rate</td>
</tr>
<tr>
<td>GDL</td>
<td>Gas diffusion layer</td>
</tr>
<tr>
<td>ICE</td>
<td>Internal combustion engine</td>
</tr>
<tr>
<td>MEA</td>
<td>Membrane electrode assembly</td>
</tr>
<tr>
<td>PEM</td>
<td>Proton exchange membrane</td>
</tr>
<tr>
<td>PEMFC</td>
<td>Proton exchange membrane fuel cell</td>
</tr>
<tr>
<td>PTFE</td>
<td>Polytetrafluoroethylene</td>
</tr>
<tr>
<td>RFP</td>
<td>Reactant flow plate</td>
</tr>
<tr>
<td>RH</td>
<td>Relative humidity</td>
</tr>
<tr>
<td>SLPM</td>
<td>Standard liters per minute</td>
</tr>
<tr>
<td>UWF</td>
<td>Uniform wall flux</td>
</tr>
<tr>
<td>UWT</td>
<td>Uniform wall temperature</td>
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## Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tbody>
<tr>
<td>$A_c$</td>
<td>Cross-sectional flow area</td>
<td>$[m^2]$</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity</td>
<td>$[J/(kgK)]$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td>------</td>
</tr>
<tr>
<td>$D_{AB}$</td>
<td>Mass diffusivity</td>
<td>$\left[ \frac{m^2}{s} \right]$</td>
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<tr>
<td>$d_h$</td>
<td>Hydraulic diameter</td>
<td>[m]</td>
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<td>$F$</td>
<td>Faraday constant (96485)</td>
<td>$\left[ \frac{C}{mol} \right]$</td>
</tr>
<tr>
<td>$f$</td>
<td>Friction factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$Gz$</td>
<td>Graetz number</td>
<td>[-]</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravity of Earth (9.81)</td>
<td>$\left[ \frac{m}{s^2} \right]$</td>
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<tr>
<td>$h$</td>
<td>Heat transfer coefficient</td>
<td>$\left[ \frac{W}{m^2K} \right]$</td>
</tr>
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<td>$h_m$</td>
<td>Mass transfer coefficient</td>
<td>$\left[ \frac{m}{s} \right]$</td>
</tr>
<tr>
<td>$H_{GC}$</td>
<td>Height of gas channel</td>
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<tr>
<td>$I$</td>
<td>Current</td>
<td>[Amps]</td>
</tr>
<tr>
<td>$i$</td>
<td>Specific enthalpy</td>
<td>$\left[ \frac{J}{kg} \right]$</td>
</tr>
<tr>
<td>$j$</td>
<td>Mass flux</td>
<td>$\left[ \frac{kg}{m^2s} \right]$</td>
</tr>
<tr>
<td>$k$</td>
<td>Thermal conductivity</td>
<td>$\left[ \frac{W}{mK} \right]$</td>
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<tr>
<td>$L$</td>
<td>Length</td>
<td>[m]</td>
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<td>$Le$</td>
<td>Lewis number</td>
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<td>--------------------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>$M$</td>
<td>Molecular mass</td>
<td>$[\frac{kg}{mol}]$</td>
</tr>
<tr>
<td>$m$</td>
<td>Blending parameter</td>
<td>[-]</td>
</tr>
<tr>
<td>$m_f$</td>
<td>Mass fraction</td>
<td>[-]</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>Mass flow rate</td>
<td>$[\frac{kg}{s}]$</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
<td>[-]</td>
</tr>
<tr>
<td>$P$</td>
<td>Total pressure</td>
<td>$[Pa]$</td>
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<tr>
<td>$Pr$</td>
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<tr>
<td>$p$</td>
<td>Partial pressure</td>
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<tr>
<td>$\bar{R}$</td>
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<tr>
<td>$R$</td>
<td>Gas constant</td>
<td>$[\frac{J}{kgK}]$</td>
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<tr>
<td>$Re$</td>
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<tr>
<td>$r$</td>
<td>Volume fraction</td>
<td>[-]</td>
</tr>
<tr>
<td>$Sc$</td>
<td>Schmidt number</td>
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<td>$Sh$</td>
<td>Sherwood number</td>
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<tr>
<td>$T$</td>
<td>Temperature</td>
<td>$[K]$</td>
</tr>
<tr>
<td>$t$</td>
<td>Temperature</td>
<td>$[^\circ C]$</td>
</tr>
<tr>
<td>$u$</td>
<td>Velocity</td>
<td>$[\frac{m}{s}]$</td>
</tr>
<tr>
<td>$W_{GC}$</td>
<td>Width of gas channel</td>
<td>$[m]$</td>
</tr>
</tbody>
</table>
$V$ Voltage [$Volts$]

$x$ Mole fraction [-]

$z$ Length along the flow channel [$m$]

$z^+$ Dimensionless position for flow with a developing velocity profile [-]

$z^*$ Dimensionless position for flow with a developing temperature profile [-]

$z^-$ Dimensionless position for flow with a developing concentration profile [-]

Greek letters

$\alpha$ Thermal diffusivity [-]

$\varepsilon$ Aspect ratio [-]

$\gamma$ Shape parameter [-]

$\lambda$ Stoichiometric ratio [-]

$\mu$ Dynamic viscosity [$Pa \cdot s$]

$v$ Kinematic viscosity [$\frac{m^2}{s}$]

$\rho$ Density [$\frac{kg}{m^3}$]

$\Phi$ Interaction parameter [-]

$\phi$ Relative humidity [-]

$\omega$ Humidity ratio [$\frac{kg_v}{kg_a}$]
Subscripts

$\sqrt{A}$: based on the square root of the cross-sectional flow area

$a$: dry air

$av$: air to vapor

$c$: cross-sectional flow area

$eff$: effective

$d$: Darcy friction factor

$f$: Fanning friction factor

$fd$: fully developed

$GC$: gas channel

$H$: constant heat flux boundary condition

$H2$: hydrogen

$h$: based on the hydraulic diameter

$m$: mixture

$N2$: nitrogen

$O2$: oxygen

$s$: saturated vapor

$T$: constant surface temperature boundary condition

$v$: vapor (or water vapor)

$va$: vapor to air

$w$: water
ACKNOWLEDGEMENTS

First and foremost, I would like to thank my supervisor, Dr. Mina Hoorfar, for her guidance and expertise throughout both my undergraduate and graduate endeavors. She has been an invaluable source of inspiration and encouragement.

I would also like to thank my committee members and all of my other educators throughout the years whom I have learned from immensely, as well as my colleagues whom I have enjoyed working alongside in the lab.

I would like to thank my family for their continued love and support. I am forever grateful for their generous time and compassion.

Lastly, I would like to thank my partner for being there every step along the way, forward or backward. The journey would not have been the same without you. Words cannot describe my appreciation for her endless insight.
DEDICATION

This thesis is dedicated to future generations, who deserve a cleaner environment in which to live and thrive. Let our efforts today pave the way for tomorrow.

Out beyond ideas of wrongdoing and rightdoing,
there is a field. I’ll meet you there.

When the soul lies down in that grass,
the world is too full to talk about.
Ideas, language, even the phrase “each other” doesn’t make any sense.

~ Rumi ~

(as translated by Coleman Barks)
CHAPTER 1: INTRODUCTION

Proton exchange membrane fuel cells (PEMFCs) have emerged as a leading alternative to internal combustion engines (ICEs), with many of the major automotive companies investing in their development and production [1, 2]. With a high efficiency and zero emissions, hydrogen-fueled PEMFCs have the ability to replace conventional technologies and drive our future society to produce power in a more sustainable manner. This push for a ‘hydrogen economy’ is imminent and provides us with an opportunity to pave the way to a cleaner future. A PEMFC is an electrochemical device that combines a fuel (hydrogen) and an oxidant (air) to create electricity, with water and heat as its only by-products. A PEMFC consists of two electrodes (anode and cathode) separated by a polymer electrolyte. The electrodes are comprised of a platinum catalyst, a porous diffusion media, and a flow plate. The reactant gases are transported from the flow plates through the diffusion media to the catalyst, which is where the reaction occurs.

As one of the most promising energy options for lowering carbon emissions, the commercialization of fuel cells is pertinent. However, in order to become an abundantly available power generation device, the cost of fuel cells must reach a competitive level with oil- or coal-based power generation. The advantages of a transition to cleaner energy alternatives, however, are invaluable. The environmental effects of burning hydrocarbons are visible in several ways, from smog choking major world cities due to tailpipe pollution, to the bleaching of coral reefs in our oceans due to rising water temperatures and acidification [3, 4]. The gradual change in Earth’s climate due to the greenhouse gas effect is melting our polar ice caps and creating positive feedbacks for continued warming [3, 4]. If our society’s thirst for depleting non-renewable oil reserves is not quenched, further environmental consequences may prevail.
Fuel cells are well-suited to replace contemporary portable and stationary power generation devices. Currently, oil-consuming ICEs are the primary means for producing automotive power and are limited by the Carnot efficiency (which is governed by the temperature difference across a heat engine). Modern-day ICEs have a maximum efficiency of ~38% due to temperature constraints and mechanical friction losses [5], and they exhaust greenhouse gases. In contrast, hydrogen fuel cells have a higher practical efficiency (>50% [3]), and they exhaust only water vapor. This means that a conversion to fuel cell engines could substantially increase the pump-to-wheels efficiency of the automotive sector, while eliminating tailpipe emissions [2, 5, 6]. With innovative production and distribution of hydrogen, the well-to-pump efficiency and emissions of a hydrogen-fuelled economy could trump that of the oil-fuelled economy, producing an enhanced well-to-wheels transportation infrastructure [5, 6]. In addition, stationary coal-fired power plants could be converted to natural gas-fueled combined heat and power (CHP) fuel cell systems to provide clean energy and heat to industrial and residential buildings. With the world’s energy demand steadily increasing, all viable and sustainable energy sources (e.g., solar, wind, tidal, geothermal, nuclear, hydro, etc.) should be used in parallel to combat our energy and environmental crises.

To achieve a required power output, a series of unit cells are combined to create a fuel cell stack. Fuel cell stacks are characterized by a volumetric power density (W/L), which is the rated power of the stack divided by its volume. Each unit cell is quantified by a surface power density (W/cm²), which is the power each cell produces divided by the active area of the cell. By increasing the power density of the unit cell, the active area can be reduced while achieving the same power, which can reduce the size and ultimately the costs of fuel cell stacks. Specifically, decreasing the active area means that less platinum is required, which constitutes a principle expense in the
production of fuel cells. Alternatively, using the same active area means that less cells are needed to produce the same rated stack power, which reduces hardware and material costs. Naturally, the architecture and design of fuel cell stacks has been tailored for their specific use, whether it be portable or stationary.

A 2012 document by the United States Department of Energy (DOE) [1] implements technical plans to increase the durability and reduce the costs of PEMFCs. Since existing ICE systems cost roughly 25-35 $/kW, a fuel cell system costing approximately 30 $/kW is required to yield a competitive technology for market infiltration [1]. As such, targets were set for an 80 kW (107 hp) PEM fuel cell stack for automotive applications running on direct hydrogen (sec. 3.4, p. 17) [1]. Examples of the 2011 statuses and associated 2017 targets include the following: the high-volume production costs should be reduced from 49 $/kW to 30 $/kW, the durability should be doubled from 2500 hours to 5000 hours, and the volumetric power density should be increased from 400 W/L to 650 W/L. To address these challenges, industry and academia are striving to demonstrate sufficient durability during automotive drive cycles, as well as drop expenditures by reducing platinum usage, lowering manufacturing and material overheads, and designing cost-effective balance-of-plant components.

Despite the allure of fuel cell technology, there are primary areas in need of improvement to produce volumetric power densities and achieve costs on par with incumbent technologies. One major issue inherent in current PEMFCs is ineffective water management [3, 7-10]. If the water produced in the reaction is not properly removed, liquid water can flood the cell and impede reactant transport to the catalysts, which decreases cell performance. However, if too much water is removed, the polymer electrolyte can become dry and reduce proton conductivity, which also decreases cell performance. Mitigation strategies to provide effective water management include
the optimization of reactant humidity levels and flow rates through the cell, along with proper design of the porous diffusion media and reactant flow plate [10, 11]. This thesis is premised on the fact that water management in a PEMFC varies spatially across the active area of a cell from the inlet to the outlet. It aims at developing an experimental technique capable of capturing the mechanisms of water removal inherent in an operational PEMFC.

Section 1.1 will describe the principles of PEMFC operation, and will review the structure and function of its fundamental components. It will also explain the various losses that can occur and elucidate their effects on PEMFC performance. Section 1.2 will identify the key aspects of water management and relate its importance to cell performance. Section 1.3 will review the literature that is relevant to this research. It will examine in-situ characterization studies and highlight recent efforts made to evaluate water removal through the GDL. Section 1.4 will outline the research objectives of the current study, while Section 1.5 will describe the approach taken to obtain the research goals. Finally, Section 1.6 will stipulate the general structure of the thesis.

1.1 PEM Fuel Cells

A PEMFC is an electrochemical device that is used to convert chemical energy into electrical energy. PEMFCs commonly use hydrogen as a fuel and air as an oxidant, and only produce water and heat as by-products. Figure 1-1 displays a schematic of a PEMFC. The polymer electrolyte, or proton exchange membrane (PEM), is located between the anode and cathode electrode. Each electrode is comprised of a platinum catalyst layer (CL) coated on the PEM, a porous diffusion media known as a gas diffusion layer (GDL), and a reactant flow plate (RFP). The RFP contains a flow field that is backed against the GDL to supply the reactant hydrogen fuel, or oxidant air, to its electrode. The reactant gases are transported from the flow fields in the RFPs through the GDLs to the CLs on either side of the PEM.
A PEMFC produces electricity through the electrochemical reduction-oxidation (redox) reaction of hydrogen and oxygen. Hydrogen is split into protons and electrons by the anode’s CL. This is called the hydrogen oxidation half reaction or HOR (Equation 1.1). The protons are transported from the anode to the cathode through the PEM and the electrons are collected as they conduct back through the anode GDL and RFP. The electrons pass through an external circuit from the anode to the cathode, which provides electrical power to a load. The electrons then travel through the cathode RFP and GDL to the cathode’s CL. Here, the electrons combine with the protons that have passed through the PEM and the oxygen that has diffused through the cathode GDL, which completes the reaction and forms water. This is called the oxygen reduction half reaction or ORR (Equation 1.2). The overall reaction describes the combination of the two half reactions where hydrogen and oxygen combine to create water (Equation 1.3).

HOR: \[ 2H_2 \rightarrow 4H^+ + 4e^- \] \hspace{1cm} (1.1)

ORR: \[ O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \] \hspace{1cm} (1.2)

Overall: \[ 2H_2 + O_2 \rightarrow 2H_2O \] \hspace{1cm} (1.3)
The theoretical open circuit voltage (OCV) that is produced from the hydrogen-oxygen redox reaction is 1.23 V at 25°C [3]. In theory, this voltage should remain constant as current is drawn from the cell. In reality, four main losses (i.e., internal current, activation, ohmic, and mass transport losses) can occur in the system and, as a result, the cell voltage drops as current is drawn [3]. Initially, internal current losses reduce the OCV from its theoretical potential and are due to electrical shorts through the PEM and/or hydrogen crossover from the anode to cathode. Activation losses are prominent at low current densities and are due to inefficiencies in the redox reaction. Ohmic losses are prominent at mid-range current densities and are due to proton resistance in the PEM and electrical contact resistances in the cell. Mass transport losses are prominent at high current densities and are due to deprivation of reactants and insufficient removal of products. The theoretical efficiency of a PEMFC can be defined as $\eta = V / 1.254$ using the lower heating value of hydrogen [3]. Therefore, these voltage losses decrease the efficiency of the cell and limit the power output. The losses are characterized by the polarization curve, which illustrates the voltage decrease as current is drawn from the PEMFC, as well as the resulting power output ($P = V \cdot I$). See Figure 1-2 for an example of a polarization curve, illustrating the four main losses.

![Figure 1-2. Example polarization curve](image_url)
Before explaining the main losses further, the layers that are integral to the operation of the PEMFC will be described. The PEM is a polymer electrolyte made of a per-fluorocarbon sulfonic acid (PFSA) ionomer that is used to transport the protons from the anode to the cathode. Nafion® by DuPont is the best-known PEM and is considered an industry standard [12]. It consists of a fluorinated polyethylene backbone (or polytetrafluoroethylene (PTFE)) with a sulphonic acid group (SO$_3$H) ionically bonded to the side chain of the copolymer [12]. The PTFE backbone provides chemical durability and mechanical strength to the membrane, while the sulphonic acid provides proton conductivity to the membrane. The SO$_3^-$ ions allow the H$^+$ ions (protons) to move through the membrane. The hydrophilic sulphonic acid regions in the membrane allow water to be absorbed into the overall hydrophobic PTFE material. Within the well-hydrated regions of the membrane, the protons are able to readily move along the sulphonated side chains [3, 12]. The proton conductivity is highly dependent on the PEM’s water content, with a high water content leading to higher proton conductivity [3, 12].

The CL is a carbon-supported platinum layer coated on either side of the PEM. A three-phase boundary is created at the CL. At this boundary, three conditions are critical for the reaction to occur: the reactant gases must have access to the platinum surface, there must be ionic contact to the PEM for the protons to travel, and there must be electrical contact to the GDL for the electrons to conduct [3, 12]. By supporting smaller platinum particles on larger carbon particles, a higher electrochemically active surface area is obtained. The carbon particles allow for electrical contact to the GDL, while a Nafion® solution is commonly added to provide ionic contact to the PEM [3, 12]. The techniques and ratios used for catalyst coatings are proprietary among manufacturers. When a CL is applied to either side of the PEM, it forms a catalyst coated membrane (CCM).
The GDL is a porous transport layer that allows for the diffusion of reactant gases from the flow field to the CL, improves the electrical connection and heat dissipation between the CL and RFP, and provides structural support for the PEM [13]. The GDL also plays a significant role in the management of water produced at the cathode by the redox reaction. As described by Mathias, Roth, Fleming, and Lehnert (2003) [14], GDLs are commonly made from a fibrous, paper-based material, which is composed of machine laid carbon fiber strands (diameter ~7 µm) that are bound together using a thermosetting polymer resin. The resin is cured through a carbonization process that is induced by heat-treatment. A carbon or graphite powder can also be added to the thermoset resin during the manufacturing process [14]. Both the carbonized resin and the carbon powder decrease the bulk resistance of paper-based GDLs.

A PTFE coating is often applied to the GDL, which helps prevent the GDL pores from flooding by making the carbon strands of the GDL hydrophobic. A microporous layer (MPL), which consists of a carbon black powder and PTFE solution, can also be added to one side of the GDL. The MPL-coated side of the GDL is placed against the CL in order to enhance electrical contact between the layers, enhance gas distribution, and improve water management. Research has repeatedly demonstrated that treating the GDL with an optimal amount of PTFE and applying an MPL to the GDL significantly decreases ohmic and mass transport losses, which ultimately increases PEMFC performance [7-10, 15-17]. A GDL is placed on either side of a CCM to form a membrane electrode assembly (MEA).

The flow field in the RFP generally contains rectangular channels, which allow the reactant gases to flow to the CL, and lands, which contact the GDL in order to conduct electricity and heat. Flow fields come in various configurations, with the predominant types being parallel, serpentine, and interdigitated. The flow field dimensions are imperative to achieving optimal fuel cell
performance. The open area (width) of the channel allows gas to readily diffuse through the GDL. However, if the channels are too wide, the GDL can bow into the channels and lose contact with the CL. Similarly, wider lands will enhance the electrical contact between the GDL. However, if the lands are too wide, the exposed area of the reactant will be reduced and can facilitate pooling of liquid water under the lands [18]. The depth and width of the channel will also influence the velocity of the reactant gas in the channel, which affects water removal characteristics [19-21]. Hydrodynamic considerations, as well as heat and mass transfer correlations, for air flowing through a rectangular channel are reviewed in detail in Chapter 4.

The PEM, CL, GDL, and RFP all have implications for the voltage losses that can occur in the cell. The ohmic and mass transport losses are the losses of primary interest to this study. In regards to ohmic losses, the proton conductivity of the PEM increases as its water content increases. Therefore, a dry PEM can increase ohmic losses. Insufficient pressure between the lands of the flow field and the GDL, or between the MPL and CL, can also increase ohmic losses by increasing contact resistance. In regards to mass transport losses, ineffective water removal leads to a phenomenon known as flooding, where liquid water will accumulate in the GDL and hinder reactant transport to the CL. Flooding is most likely to occur under the lands of the flow field, but can extend throughout the entire GDL if there is insufficient water removal in the channels [18]. Finally, a higher flow rate in the RFP will lead to a higher reactant concentration gradient from the channel to the CL, thereby increasing reactant transport and reducing the effect of mass transport losses [3, 22-24]. Hence, the properties of the MEA, the design of the RFP flow field, and the cell conditions can all greatly affect the occurrence of voltage losses.
1.2 Water Management

Several mechanisms govern water management in an operational fuel cell. In addition to the water produced at the cathode from the redox reaction, the protons crossing the membrane drag water from the anode to the cathode in a process known as osmotic drag [3, 12]. The concentration gradient from the cathode to the anode will drive the accumulated water backward through the membrane in a process known as back diffusion [3, 12]. If the pressure differs in the cathode and anode channels, liquid water can also hydraulically permeate through the membrane [3, 12]. Any excess water must be effectively removed from the cathode’s CL and GDL to avoid flooding. This can be achieved by water vapor diffusion through the GDL and convective mass transport in the air flow channels. These interrelated processes are predominantly influenced by the relative humidity (RH) of the air input and the flow rate (FR) of the air in the channels. In particular, drier air and faster flow rates will cause a higher rate of water vapor removal [25].

Water vapor that is removed from the cathode’s CL must transport through the MPL before entering the carbon fiber substrate of the GDL and subsequently the flow channels. Since most MPLs have a high capillary pressure, vapor transport is the main mechanism of water removal in the MPL. If the RH in the flow channel is low, water will transport through the GDL to the flow channel in vapor phase. However, as the reactants becomes more humid, condensation is prone to occur. If the GDL has a low thermal conductivity, the increased temperature drop can cause water vapor to condense in the substrate pores, especially under the lands of the flow field. The MPL creates a hydrophobic barrier between the CL and GDL in order to prevent liquid water from flooding backward to the CL [26]. Capillary forces drive liquid water transport through the GDL and into the flow channels where gas shear removes the droplets. Insufficient water vapor removal through the GDL and MPL can cause condensate to pool and lead to flooding in the CL. Cracks in
the MPL can facilitate liquid water transport through the GDL. However, if proper water management techniques are not employed, liquid water can accumulate in the GDL and hinder diffusion of oxygen to the areas of the CL under the lands. Further, liquid water can saturate the CL and completely block oxygen transport to the reaction sites. Flooding in either the GDL or CL greatly reduces PEMFC performance [26].

It is important to note that water transport varies along the length of the flow channels. For example, partially humidified air is commonly input into the flow channels in order to keep the PEM hydrated. As the air flows down the channels and removes excess water, the water content in the air increases. As the air becomes fully saturated, its water removal capabilities become limited in the latter part of the channels, which can lead to down-channel flooding [27]. Alternatively, air with a lower RH can be input into the flow channels to decrease the likelihood of flooding near the outlet [28]. However, this can cause a high rate of water removal up-channel, which can dry out the PEM near the inlet. Either extreme can hinder performance by causing water and current imbalances in the cell that can lead to accelerated degradation of the PEM. Hence, understanding the mechanisms of water vapor diffusion in the GDL and mass convection in the flow channels is critical to mitigating potential losses caused by ineffective water management.

1.3 Literature Review

This section will discuss experimental and theoretical studies that have examined the effect of input air conditions on in-situ PEMFC performance. It will then review prominent efforts made toward understanding water removal characteristics of the GDL and flow field.

1.3.1 In-situ performance

Cathode input conditions have repeatedly been demonstrated to affect fuel cell performance [18, 22, 27-33]. Yan, Toghiani, Liu, and Wu (2005) [22] tested the effect of a variety
of cathode air inputs on cell performance, including RH and flow rate. Regarding RH, results indicated an increase in cell performance corresponding to an increase in the cathode air RH. Regarding flow rate, mass transport losses were apparent at a lower current density for a low oxygen stoichiometry (i.e., stoichiometry of 2). However, above an oxygen stoichiometry of 4, increasing the air flow rate only marginally improved cell performance. The differences in limiting current across flow rates may be due, in part, to differences in oxygen starvation given that lower flow rates cause a greater drop in the reactant concentration in the latter part of the channel.

In a subsequent study, Yan, Toghiani, and Wu (2006) [29] investigated the effects of water transport on cell performance by condensing the output reactants and measuring the net drag coefficient, which is defined as the net number of water molecules transported through the membrane per proton from the anode to the cathode. They found that for a cell running at 80°C with a fully humidified anode, increasing the cathode air input RH generally decreases the net drag coefficient. This outcome might be expected given that more humid cathode air inputs are less capable of pulling water from the anode. Results further indicate that as the current density increases, there is a decrease in the net drag coefficient as the produced water begins to back-diffuse from the cathode to the anode. Since this study used a 183 μm thick PEM (Nafion 117), the primary cause of poor performance for dry air inputs was insufficient hydration of the membrane on the anode side due to a lack of back diffusion, which yielded high ohmic losses. Accordingly, a thinner membrane may retain a higher water content for similar input conditions as it would experience less resistance to back diffusion [30].

Chen and Chang (2013) [31] tested the performances of GDLs with varying MPL properties for a series of cathode RH levels using a cell with a serpentine flow field. The cathode air humidity levels ranged from 13.61% (dry) to 100% (fully humidified). The cell temperature
was kept at 70°C, the anode was kept fully humidified, and the flow rates of the gases were kept constant among the tests. In accordance with the above findings, results demonstrated a continual increase in the peak power density from dry to saturated cathode RH inputs across all MPL variations. Notably, increasing RH does not always result in an increase in performance. Santarelli and Torchio (2007) [28] found that the effect of humidification is dependent on other factors such as cell temperature and current density. For example, for high current densities, which yield a high rate of water production, and low cell temperatures (50°C), which hinder water evacuation, saturated RH inputs (100%) can decrease performance by causing flooding.

Natarajan and Nguyen (2005) [27] used a cell with an electrode that is segmented along the length of a single parallel gas channel to find the local current density distribution. They found that, for fully humidified reactant streams, decreasing the air flow rate negatively affected the current density downstream. The faster flow rates increased the availability of oxygen, especially in the latter sections of the gas channel, which resulted in improved cell performance. However, even at high flow rates, the current density still fluctuated and decreased down-channel for humidified gas streams. For dry air streams, on the other hand, the current density remained more stable in the latter parts of the channel. Hence, they concluded that increasing the RH of the inlet air results in liquid water accumulation downstream, which reduces performance.

Oberholzer and Boillat (2014) [18] evaluated the water content throughout a PEMFC for two reactant RH conditions using high resolution neutron imaging. A differential fuel cell, which is a scaled-down version of a larger cell that flows gas at a high stoichiometric rate, was used to mimic the local conditions of a full-size fuel cell. Radiograms revealed the water distribution in the anode and cathode flow field and GDL, as well as the PEM. As expected, when both reactants were input at 90% RH, the cathode GDL contained a higher water content than when a fully
humidified hydrogen input (100% RH) and completely dry air input (0% RH) were used. For the 90% RH condition, liquid water accumulation was concentrated underneath the lands at lower current densities while the rest of the cathode GDL remained dry. During higher current densities, the entire GDL and flow channels became flooded with liquid water. In contrast, for the 100% RH hydrogen and 0% RH air condition, the increase in water content occurred at a higher current density and to a lesser extent, accumulating only in the areas underneath the lands.

Theoretical analyses provide support for the experimental findings discussed above. Jamekhorshid, Karimi, and Noshadi (2011) [32] proposed a two dimensional, partially flooded GDL model to examine the effects of cathode inlet humidity, among other cell operating parameters. The model demonstrates that the total current density is directly and positively influenced by increases in the inlet RH of the cathode air. However, higher cathode RH are shown to increase the likelihood of flooding, as well as accelerate its occurrence. For cathode RH levels below 60%, flooding is unlikely to occur. However, with each increase in RH above 60%, the onset of flooding is predicted at an earlier location along the channel. This model also demonstrated that higher cathode air flow rates can delay, and even prevent, liquid water accumulation, which is consistent with experimental outcomes. An algorithm presented by Guvelioglu and Stenger (2007) [33] revealed similar results, with a higher air RH and lower air flow rate predicting down-channel flooding. Both of these studies found an exponential decrease in the local current density along the channel length from the inlet to the outlet.

1.3.2 Water removal characteristics of the GDL and flow field

Prior research has investigated the relationship between input conditions and water removal rates through the GDL and flow field. Most of these studies are derived from standard water vapor transport test methods used in the textile industry (also classified as water vapor transmission,
resistance, or permeability) [34]. These methods involve placing heated water above or below a textile sample and measuring the rate of water transport through the layer. A review and comparison of these test methods can be found elsewhere [34]. One method in particular is called the “Sweating Guarded Hot Plate Test Method” (ISO 11092) [35], in which water is placed on a heated plate below a textile and partially humidified air is fed over the sample at 1 m/s. Chun et al. (2011) [36] developed a home-made testing apparatus to measure the water vapor permeability of GDLs with MPLs of varying levels of hydrophobicity. They placed a 7 cm diameter GDL sample over 70°C water and input 65°C dry nitrogen gas at 1 liter/min into a single channel above the GDL. The humid output nitrogen was condensed and weighed to find the water vapor permeability of the GDLs.

Dai et al. (2008) [37] measured the water transport flux through a GDL-PEM-GDL combination, and subsequently through GDLs with MPLs (2009) [38]. They used fuel cell test hardware with an active area of ~50 cm² (7 x 7 cm) and a cell temperature of 70°C. A single channel serpentine anode flow field was used to flood one side with water, while a dual channel serpentine cathode flow field was used to flow 70°C air at different inlet flow rates and levels of relative humidity on the other side. The outlet air was condensed, and the water flux through the PEM and GDLs was found by subtracting the known water content of the inlet humid air from the water collected in a reservoir, while accounting for any water vapor in the condenser exhaust air. The water vapor in the condenser exhaust air was found using a thermocouple to find the saturation pressure of the fully humidified exhaust.

Results from these two studies [37, 38] indicate that increasing the RH of the air input decreases the water flux across the layers. For GDLs with MPLs, using both dry and humid air inputs, increasing the flow rate results in a logarithmic trend. That is, there is an initial increase of
the water flux at lower flow rates, which is followed by a leveling out at higher flow rates. The researchers correlated the water fluxes for different inputs with equivalent water production rates of an operational fuel cell. They identified a region for which the combination of input conditions produced fluxes that were similar to production rates at equivalent current densities, indicating an ideal water balance and therefore an optimal operating zone. With an oxygen stoic. of 2, the optimal zone encompassed an operating current density range of 0.5 to 1.1 A/cm² when feeding 64% RH air, and an operating range of 1.1 to 1.5 A/cm² when feeding 40% RH air. They concluded that there is a greater potential for flooding or drying outside of this zone.

Quick, Ritzinger, Lehnert, and Hartnig (2009) [39] characterized the water transport through GDLs using modified 50 cm² fuel cell test hardware at 54.5°C. A serpentine channel was flooded with water, while dry air was fed through a parallel flow field. The water and air side were separated by a CCM, with a hydrophilic layer on the water side and a GDL on the air side. The rate of water transport was found by measuring the water loss in a reservoir. They reported an effective diffusion coefficient, but neglected the effect of convective transport in the channels and transport resistance of the CCM (i.e., essentially reporting an overall mass transport resistance), which makes this quantity unsuitable for comparison with other studies. They correlated the water removal rates to in-situ performance using dry operating conditions and found that a high water transport rate can lead to drying of the PEM and reduce performance due to the increased ohmic resistance of the PEM.

Bresciani, Casalegno, Varisco, and Marchesi (2014) [40] also used a similar setup to that used above [39] to characterize the water vapor diffusion and liquid water permeation through the GDL. The GDL was placed between two triple serpentine distributors with a 42 x 42 mm exposed area with pressurized water on one side and dry input airflow on the opposite side. The water side
inlet was attached to a water column to create a hydrostatic pressure while the water outlet was dead-ended. Using pressures below the capillary pressure of the GDL, they found the water vapor diffusion rates by using an RH sensor at the outlet of the air side. Once accounting for the channel mass convection, the authors report an effective water vapor diffusion coefficient for a GDL (with MPL) of 0.029 cm$^2$/s at 40°C, 0.033 cm$^2$/s at 60°C, and 0.053 cm$^2$/s at 80°C.

In addition to a vapor gradient, a temperature gradient across the GDL (from CL to flow field) caused by the heat produced at the cathode’s CL can also drive diffusion. Owejan et al. (2010) [26] used a 50 cm$^2$ water-flooded hydrophilic mesh flow field and serpentine air flow field to study the rate of diffusive transport through a PEM and GDL with MPL driven by the inlet air RH and an induced temperature gradient. The liquid water side was held at 80°C and air was fed at 50% or 100% RH with air temperatures of 0, 4, or 8°C lower than the water temperature (i.e., 80, 76, 72°C, respectively). The output humid air was condensed and the collected condensate was used to quantify the water transfer rate. For the 50% RH input, they found similar transport rates across all temperature gradients. These rates were well above an equivalent in-situ water generation rate at 1.5 A/cm$^2$. However, for the 100% RH input, no significant water transport was found when there was a lack of temperature gradient (i.e., 0°C). The rate increased to an equivalent in-situ water generation rate of 1 A/cm$^2$ for the 4°C gradient and 1.5 A/cm$^2$ for the 8°C gradient. Liquid water permeation of GDLs with varying MPLs was measured and in-situ performance testing was conducted using a series of test conditions. Based on their combined results, they conclude that concentration-driven water vapor transport induced by both vapor and thermal gradients are the primary water removal mechanisms on the cathode.

Studies have used a mass exchanger system to find the water vapor transport across a GDL. In essence, these studies feed a humid air stream and a cocurrent dry air stream on either side of a
GDL to exchange water vapor through the GDL. The streams are input at the same flow rate to avoid pressure driven flow from one channel to the next. They use RH sensors at the inlets and outlets to determine the water flux across the GDL. Casalegno, Colombo, Galbiati, and Marchesi (2010) [41] determined the global coefficient of water transport based on the obtained flux and logarithmic mean concentration difference, using plates with triple serpentine flow fields. In a successive study, Casalegno, Bresciani, Groppi and Marchesi (2011) [42] apply the convective mass transport coefficients of the channels to separate the GDL water vapor diffusion coefficient from the global transport coefficient. They report an effective diffusion coefficient for a GDL with MPL of 0.0556 cm$^2$/s at 60 °C.

Similarly, LaManna and Kandlikar (2011) [43] used a mass exchanger setup to find the effective water vapor diffusion coefficient of the GDL using a 1 x 1 mm single parallel channel. An analytical model was presented in order to extract the diffusion coefficient using the measured inlet and outlet RH levels of both channels, as well as the convective mass transport coefficient of the channels. They reported effective water vapor diffusion coefficients ranging from 0.026 – 0.148 cm$^2$/s at 25 °C for various GDLs with and without MPLs [43, 44]. Collectively, these studies [36-44] provide insight into the pure effect of the diffusive water vapor resistance of the GDL.

As mentioned, these designs are analogous to designs for standard methods of measuring water transport through textile fabrics. However, some studies only report an overall or global water resistance. There remains a gap in the literature to accurately separate the mass transport convection in the channel(s) from the GDL water vapor diffusivity. This is, in part, due to the scarcity of correlations for convective mass transport coefficients of developing flow in rectangular channels. The majority of the studies use serpentine channels [37-42], in which other mechanisms of water removal may be present (e.g., convection of air through the GDL). Also, all
of the studies mentioned [36-44] use only the inlet and outlet conditions to quantify mass transport, and can only predict the water concentration profile along the length of the channel based on first principles. Finally, the studies that have attempted to link pseudo experimental techniques to in-situ performance have used input conditions that were inconsistent between experiments, which hinders comparison [36, 39, 26]. While the studies described above provide valuable insight into water management aspects in PEMFCs, limited research has explicitly studied the effect of water removal rates on in-situ cell performance using comparable test conditions.

1.4 Research Objectives

In sum, research has identified that water produced at the cathode must be effectively managed in order to achieve optimal fuel cell performance. Cathode air inputs are known to drive water vapor diffusion in the cell and govern local water removal capabilities along the length of the flow field. Hence, varying these inputs can substantially affect in-situ fuel cell performance. For example, a dry air input and fast velocity of air in the flow field channels will cause a high rate of water removal to occur at the beginning of the flow field. If this rate exceeds the rate of water production, the PEM can potentially become dry near the channel inlet and lead to increased ohmic losses in the cell. As the air continues down the channel and becomes more humid, the rate of water production may overcome the rate of water removal. Past this point, down-channel flooding of the GDL can occur, which will hinder oxygen diffusion and lead to increased mass transport losses. Both of these situations result in decreased fuel cell performance.

The primary objective of this study is, therefore, to determine the local rates of water removal through the GDL along the length of the flow field across a variety of air inputs and relate these results to in-situ performance using the same air inputs for the cathode. In order to achieve this, an experimental setup was designed that was capable of both characterizing in-situ
performance and determining the water removal capabilities within a quasi-operational fuel cell. The two water removal processes of interest were water vapor diffusion in the GDL and mass convection in the flow field, which are driven by the air input RH and flow rate, respectively. By comparing the results, we anticipate a correlation between the water removal rates obtained from the in-situ and quasi-operational fuel cell experiments. This relationship will provide valuable insight into water management aspects in PEMFCs and will help to predict operational conditions that will yield stable performance at high power densities.

1.5 Research Approach

Two sets of test plates and one set of coolant plates were designed and manufactured for the purposes of this study, as well as for use in concurrent and future studies. One set of test plates consisted of two reactant flow plates and the other set consisted of an air flow plate and a segmented water plate. Two analogous experiments were conducted using these two sets of test plates that were interchangeable within a common test cell. The first type of experiments involved supplying hydrogen and air to an MEA via the two RFPs, and measuring the in-situ performance as a function of two cathode air inputs: the inlet air relative humidity and the inlet air flow rate. This experiment will be referred to as the in-situ experiment. Two flow rates, low and high, and four relative humidity conditions, ranging from dry to oversaturated, were tested. In an effort to isolate the effect of the cathode-side inputs on in-situ performance, the anode inputs and cell temperature remained constant. Electrochemical testing was used to characterize the in-situ performance and results were compared across input conditions.

The second type of experiments involved replacing the two reactant plates with the air flow plate and segmented water plate. The air flow plate replaced the cathode-side reactant plate, while the water plate was used to flood the MPL side of a GDL, simulating a flooding condition. The
water plate was segmented such that the rate of water removal through the GDL could be captured along the length of the flow field. This experiment was designed to mimic the mechanisms of water removal during in-situ operation (i.e., water vapor diffusion through the GDL and mass convection in the flow field). Hence, the cathode-side conditions that were used for the in-situ testing in the first type of experiments (described above) were also used as the air-side conditions in the second type of experiments. In particular, identical input air RH levels and flow rates were tested, the flow geometry of the RFP was retained in the air flow plate, and the cell temperature remained constant. In addition, the GDL was taken from the same sheet as that of the cathode-side GDL used for the in-situ MEA. Due to its operational commonalities with the in-situ experiment, this experiment will be referred to as the quasi in-situ experiment.

The coolant and test plates were contained within a custom test cell using a design that was derived from a parallel plate heat exchanger system [25]. This design is regularly used in fuel cell stacks and standard test cell arrangements. For the in-situ experiment, this design directs the reactant hydrogen and air to the RFPs. In order to keep the cell isothermal for testing, the two coolant flow plates are backed against the test plates and water is supplied at a controlled temperature. The reactant and coolant fluids are directed from a common manifold to their respective plates via openings in the flow geometry. In order to prevent fluid leakage, the plates are bordered with gaskets and are compressed between two backing plates. For the quasi in-situ experiment, this design directs air to the air flow plate, while water is input to the individual sections of the segmented water plate. The test cell is housed within a test station, which communicates with a desktop computer to control the gas input conditions.

The results of the quasi in-situ experiment will be related to the in-situ performance by comparing the rate of water removal along the length of the flow field for each condition with
performance fluctuations among the chosen inputs. Since these two types of experiments closely resemble one another and isolate the cathode-side inputs, the quasi in-situ water removal data can be used to infer the reasons for fluctuations in the in-situ fuel cell performance across test conditions, providing insight into water management in PEMFCs.

1.6 Structure of Thesis

This thesis is comprised of seven chapters. Chapter 1 provides a brief introduction about PEMFC technology. It describes the fundamental principles for operation, as well as the key components and their functions within the cell. It also describes the water removal mechanisms that occur within the cell and explains how poor water management can lead to electrochemical losses during in-situ operation. In addition, it provides a review of the efforts that have been made to study the effect of air inputs on water removal capabilities and in-situ performance. This chapter concludes with a definition of the research objectives and an overview of the research approach. Chapter 2 introduces the experimental setup, outlining each component and describing each subcomponent in detail. Chapter 3 explains the experimental methods that were used for testing in both the in-situ and quasi in-situ experiments. Chapter 4 provides a detailed review of the governing equations for heat and mass transfer of laminar flow in a rectangular channel. Chapter 5 presents an analytical model that was created to extract the effective water vapor diffusion coefficient of the GDL from the experimental data. Chapter 6 reports the results from the two types of experiments and discusses their implications. Chapter 7 provides a summary of the findings and highlights the contributions of the project, including suggestions for future directions.
CHAPTER 2: EXPERIMENTAL SETUP

A schematic of the complete experimental setup is shown in Figure 2-1. The major components of the setup are (1) the test station, (2) the test cell, (3) the test plates, and (4) the output air condenser. The test station (described in Section 2.1) is used to control the input conditions and house the test cell, which is inverted and suspended horizontally. The test cell (described in Section 2.2) is covered in an adhesive, reflective thermal insulation and consists of compression hardware, a fluid distribution network, and a coolant system. The in-situ and quasi in-situ sets of test plates (described in Section 2.3) are interchangeable within the peripheral components of the test cell and contain the MEA and GDL, respectively. The output air condenser (described in Section 2.4) is used to evaluate the water content of the output air. The following sections provide a detailed description of each of the components and subcomponents of the experimental setup.

2.1 Test Station

An Arbin fuel cell test station is used to measure the electrochemical performance and control the input gas conditions. The station is connected to a desktop computer which acts as the controller and data acquisition unit. The test station has a maximum power loading of 200 W. The user can select a low voltage range of 0 to 2 V or a high range to 12 V, and can select a low current range of 0 to 1 A, medium range to 10 A, or high range to 125 A. Nitrogen, air, and hydrogen gas are supplied to the back of the test station at the appropriate pressure from respective gas cylinders. The nitrogen is used for purging the system, while the air and hydrogen are used as the oxidant and fuel reactants, respectively. The flow rates of the air and hydrogen are controlled with independent electronic mass flow controllers. The air can be controlled from 0.2–10 SLPM and the hydrogen from 0.08–4 SLPM, with a flow accuracy of ± 1% (full scale).
Figure 2-1. Schematic of experimental setup including (1) the test station, (2) the test cell, (3) the test plates, and (4) the output air condenser.
To control the humidity level and temperature of the reactant gases, they each pass through a dew point humidifier and then a heated exit-pipe before entering the fuel cell. Extra tubing was needed to connect the gas supply lines to the test cell, and also to connect the output air-line to the condenser. To minimize heat losses, all extra tubing was wrapped in an adhesive insulation tape and then all tubes and gas fittings were covered with polyethylene pipe insulation. The gas and dewpoint temperatures are set and regulated with a proportional-integral-derivative (PID) controller, implementing OMEGA K-type thermocouples (±1°C accuracy) as sensors for temperature feedback. The relative humidity of the input gases is set by choosing the corresponding dewpoint temperature for a specific gas temperature. De-ionized water is supplied to the test station for humidification of the gases. Figure 2-1 shows the test station connected to its external components and test cell orientated within it.

2.2 Test Cell

As outlined in Section 1.5, the test cell performs three main operational functions. First, compression hardware (described in Section 2.2.1) compresses the gasket material throughout the cell to prevent fluid leakage, and holds the cell components together. Second, a fluid distribution network (described in Section 2.2.2) directs the fluids to their specific flow plates. Third, a coolant system (described in Section 2.2.3) pumps water at a controlled temperature down two coolant flow plates to keep the test plates isothermal. Figure 2-2 provides a SolidWorks rendering of the assembled test cell (containing the in-situ test plates). As noted in Figure 2-2, the outer dimensions of the test cell are 113.5 × 110 × 180 mm (height × width × length). The coolant and test plates are machined out of graphite and have an outer dimension of 6 × 61 × 151 mm. Each plate contains a flow manifold that directs the applicable fluid into a centered flow field and a gasket around the periphery to seal the fluid within its plate.
Figure 2-2. SolidWorks rendering of the assembled test cell (containing the in-situ test plates) from four viewing orientations: (a) isometric (b) top (c) side (d) front

Figure 2-3 provides two exploded cross-sectional views of the test cell. As depicted in the figure, the coolant flow plates (1) and test plates (2) are compressed between the piston backing plate (3) and the manifold backing plate (4). The piston backing plate holds the piston (5) while inlet and outlet fluid manifolds (6) are connected to the manifold backing plate. The tie bolts (7) pass through the entire assembly and hold the force of the pressurized piston. Current collectors (8) are inset within the piston top and manifold backing plate and sit flush against the coolant plates when the cell is compressed. O-rings and gaskets seal neighbouring components.
Figure 2-3. Exploded cross-section of experimental test cell (containing the in-situ test plates)

Note. Labelled components are as follows: (1) coolant flow plates, (2) test plates, (3) piston backing plate, (4) manifold backing plate, (5) piston, (6) inlet and outlet fluid manifolds, (7) tie bolts, and (8) current collectors

2.2.1 Compression hardware

The test cell’s compression hardware consists of the two backing plates, a piston, and six tie bolts. The piston backing plate has a blind cylinder cavity that holds the piston as well as threaded holes that the tie bolts screw into. The piston forms a tight fit in the cylinder cavity and is sealed with two O-rings that sit in appropriate grooves. Both the piston backing plate and piston
are made of 60-61 aluminum, for structural and thermal expansion considerations. The top of the piston extends over the piston backing plate and serves as a base for the coolant and test plates. The tie bolts sit within counterbored holes in the fluid manifold, pass through the manifold backing plate, and screw into the piston backing plate.

Both the piston top, fluid manifold, and manifold backing plate are made of 1” (25.4 mm) high-density polyethylene (HDPE) plastic, so they do not sink heat away from the test plates. The tie bolts are 3/8” 316 stainless steel socket head cap screws. Nitrogen is supplied to the bottom of the piston from a small inlet port which allows it to enter the chamber. The piston has an area of 6700 mm$^2$ and a gauge pressure of 60 psig (~414 kPa) is supplied. Since the force of the piston is distributed over the coolant and test plate area of 9211 mm$^2$ (61 × 151 mm), a pressure of ~300 kPa is applied. This pressure achieves compression of the gasket material and ensures contact between the plates as well as their respective layers.

2.2.2 Fluid distribution

The fluid distribution network consists of the inlet and outlet fluid manifolds that direct the fluids to and from the cell, as well as openings in the flow plates that guide the fluids into the flow fields. The fluid manifolds are placed on top of the manifold backing plate and contain fittings to connect the coolant and reactant gas lines. Each fluid passes through the manifold backing plate and into its own plenum in the coolant and test plates, formed by 6.35 mm through-holes. Each fluid is then directed from its inlet plenum through an opening to the inlet header in its intended flow plate. The fluid then travels down the flow field and is removed by a symmetric outlet header, plenum, and manifold on the opposite end of the flow plate. A gasket pattern was designed to prevent leakage between the plenums, while allowing the fluids to enter their appropriate headers. The gasket also borders the plate area to ensure the fluids are contained within the flow field.
Figure 2-4 provides an exploded depiction of the fluid distribution network for the in-situ experiment with concurrent reactant flow. The overall network has a “U”-shaped configuration, since the inlet and outlet manifolds are on the same side of the cell. The reactant plates and the coolant plate on the manifold side contain 6.35 mm through holes that form the plenums, while the coolant plate on the piston side is capped to plug the fluid flow. The coolant enters and exits in the center of either side of the coolant plates and, therefore, the coolant inlet and outlet remain in the middle of both fluid manifolds. The reactants, on the other hand, enter and exit on diagonally opposite corners of the reactant plates, following a “Z”-type pattern within each plate [19]. The reactant plates are identical such that, the openings for the hydrogen headers and the openings for the air headers are on either side of the coolant plenums when flipped to face one another. The locations of the reactant inlets and outlets are, therefore, reversed on the inlet and outlet manifolds.

*Figure 2-4. Flow distribution network for the in-situ experiment*

*Note. The manifold-side plates (left) are transparent to facilitate viewing*
Since the test plate gaskets are aligned during compression, round gaskets were not suitable as they could cause initial misalignment of the plates. As such, rectangular gaskets were used and gasket grooves were designed to create a flush seal between the faces of each plate. The gaskets were cut out of 3/32” (2.381 mm) silicon material using a waterjet. To prevent tearing, the material was placed between two metal sheets during cutting. To ensure that the compressed gaskets fit properly in the gasket grooves, the cross-sectional area of both the groove and the uncompressed gasket were equal. If the cross-sectional area of the gasket is larger than the cross-sectional area of the groove, the compressed gasket will lock against the walls and extend past the groove, preventing contact between the plates. This phenomenon is known as gasket locking. Conversely, if the cross-sectional area of the gasket is smaller than the cross-sectional area of the groove, the gasket will not seal against the groove wall, facilitating leakage. Since the groove was machined at a constant width of 3.175 mm (1/8”) and depth of 2 mm, and the uncompressed gasket had a thickness of 2.381 mm, the gasket width was cut at 2.667 mm. Hence, both the uncompressed gasket and the compressed gasket in the groove had a cross-sectional area of 6.35 mm², which ensured proper contact and sealing between the plates. The gasket pattern was designed such that the uncompressed gasket was centered within the groove. The final gasket compression was 16%.

2.2.3 Coolant system

The coolant system consists of a Thermo Scientific cryostat water bath (NESLAB RTE 7) with a circulation pump that cycles water to and from the coolant flow plates at a controlled temperature. The coolant flow plates have an inlet and outlet header connected to a parallel flow field. The flow field is comprised of fifteen straight channels, which are separated by fourteen lands. The channels are 2 mm wide and the lands are 1 mm wide, resulting in a total width of 44 mm. The channels run 60 mm lengthwise along the flow plate and have a depth of 4 mm. The inlet
and outlet headers also have a depth of 4 mm and consist of five tapered sections that each subdivide into three channels of the flow field. Since the coolant enters and exits at the centerline of the plate, and the flow field covers the entire width, the tapered sections of the headers help to direct an even amount of flow to the outer channels as compared to the inner channels. This was important in order to attain an even heat transfer across the test plates. See Figure 2-5 for a SolidWorks rendering of the coolant flow plate and the final manufactured plate.

![Coolant flow plate](image)

*Figure 2-5. Coolant flow plate (a) rendered and (b) machined*

The pump on the cryostat has a characteristic pump curve that describes the pressure head it can supply at a certain flow rate. The coolant flow plate has a characteristic system curve that is determined from the pressure drop that occurs across the water plate as a function of flow rate. When these two systems are connected, the point at which the system curve intersects the pump curve constitutes the final operating point. If the pressure drop in the coolant flow plate is excessively high, the operating point flow rate will be low, which may lead to ineffective heat
transfer to the test plates. To determine whether the approximate operating point was at a sufficiently high flow rate, the pump curve for 20°C, published in the cryostat manual, and the system curve of the coolant flow plate, found using COMSOL, were compared (see Figure 2-6).

The initial input flow rate that was chosen was 12 LPM, since this is close to the pump’s maximum flow rate of 15 LPM. Since the pump supplies coolant to two plates in parallel, the flow rate per plate is half the total flow rate and the pressure drop is the same for both plates. At the 12 LPM input flow rate (6 LPM per plate), the average velocity for the fifteen channels, with the 2 × 4 mm channel cross-section, is 0.833 m/s. This results in a Reynolds number \( Re = \frac{\bar{u}d_h}{\nu} \) of 2222, using a kinematic viscosity for water at 20 °C of 1×10⁻⁶ m²/s and a hydraulic diameter for the channel of 2.667 mm. This proves that the Reynolds number for this case is just less than 2300 and the flow can therefore be considered laminar.

*Figure 2-6. Characteristic system curve for the coolant plates and pump curve for the cryostat pump (at 20°C), with the operating point of the coolant system marked at the intersection*
To ensure that the design of the header and flow field geometry provides a relatively even distribution across the fifteen channels, the flow was simulated using a COMSOL laminar flow model. The 3D geometry of the water passageways in the coolant plate (i.e., the headers and flow field) was imported from SolidWorks to COMSOL, where an appropriate mesh was applied. The geometry was divided into sections, such that the mesh size could be adapted according to the size of the section. The mesh was refined until the final results converged and produced no significant changes. The final mesh consisted of 952,225 elements. This was approaching the maximum number of elements that could be solved for due to computational limits. The final model geometry and an expanded view of the mesh are presented in Figure 2-7. The inlet boundary condition was a mass flow rate and the outlet boundary condition was a constant gauge pressure of 0 Pa.

Figure 2-7. Model geometry for coolant water passageways with an expanded view of the mesh

Note. Axes values are in millimeters

Several iterations of the header geometry were modelled using a volumetric flow rate of 6 LPM (or mass flow rate of 0.0998 kg/s using a density for water at 20°C of 998 kg/m³) in order to find an acceptable flow distribution [45]. Once an acceptable header geometry was found, the model was used to find the pressure drop across the flow geometry using input flow rates of 1.5,
3, 4.5, and 6 LPM. This data formed the characteristic system curve for the coolant plates that is plotted in Figure 2-6. As can be seen in this figure, the final operating point is ~10.75 LPM, with an estimated pressure drop of 20,410 Pa from the system curve. The flow rate at the operating point was considered suitable, as it was on the higher end of the pump’s flow rate. Thus, the model was re-solved at the operating point flow rate of 5.375 LPM (or 0.0894 kg/s using a density for water at 20°C of 998 kg/m³). The velocity field and pressure distribution at a surface plane cut horizontally along the midpoint depth of the channels are presented in Figure 2-8. The final average velocity in the channels was 0.7465 m/s, which resulted in a Reynolds number of 1991. The final pressure drop from the model was 20,429 Pa, which is comparable to the estimated pressure drop. The final flow distribution among the 15 channels was modest, deviating a maximum of ±40% from the theoretical average flow rate of 0.358 LPM per channel (see Figure 2-9).

Figure 2-8. Surface map of (a) velocity field and (b) pressure distribution for the coolant plate

Note. Axes values are in millimeters
Figure 2-9. Flow distribution across the 15 channels of the coolant plate at the operating point

2.3 Test Plates

To reiterate from Section 1.5, there are two sets of test plates. The first set is for the in-situ experiment, and is explained in Section 2.3.1. This set consists of two duplicate RFPs, which have an 8 cm² parallel flow field. These plates are used in the test cell to characterize the in-situ electrochemical performance of the operational fuel cell. The second set of test plates is for the quasi in-situ experiment and is explained in Section 2.3.2. This set consists of an air plate, which has flow geometry identical to the in-situ reactant plate, and a water plate, which has a matching active area that is segmented into five sections along the length of the flow field. Each of the five sections of the water plate is connected to a water column. These plates are used in the test cell to characterize the quasi in-situ performance of the GDL and flow field. Like the coolant plates, the test plates are fabricated out of 6.35 mm (1/4”) thick graphite plates that are 61 mm wide and 151 mm long. The following sections provide a detailed description of each of the test plates used for the in-situ and quasi in-situ experiments.
### 2.3.1 In-situ

For the in-situ experiment, the RFPs are located between the two coolant plates and are used for both the anode and the cathode. They direct the reactant gases to the electrodes’ active area and provide electrical contact between each electrode’s GDL and flow field lands. Two brass plates, each with one side coated in gold, are used as the current collectors. The gold-coated side of each current collector is backed against the coolant plate of either electrode and electrical lugs are attached via a pick-up location. A dummy GDL is placed between the backs of the RFPs and the lands of the coolant flow plates, as well as between the backs of the coolant flow plates and the current collectors, in an effort to minimize contact resistance between the layers and facilitate electrical conductivity.

*Reactant flow plate*

The RFPs have an inlet and outlet header connected to a parallel flow field. The flow field is comprised of nine straight channels that are separated by eight lands. The channels are 1.588 mm (1/16”) wide and the lands are 0.839 mm wide, resulting in a total flow field width of 21 mm. The length of the flow field is 38 mm, which results in an active area of 7.98 cm² (or ~8 cm²). Within the active area, the channel depth is 0.5 mm. The inlet and outlet headers have a depth of 4 mm, and consist of three tapered sections that each subdivide into three straight channels. These channels link the headers to the flow field, and their depth transitions accordingly. The tapered sections of the headers help to achieve an even flow distribution among the nine channels, which was important in order to attain a proper current distribution across the width of the active area. See Figure 2-10 for a SolidWorks rendering of the RFP and the final fabricated plate.
As can be seen in Figure 2-10, there is an outer and inner section to the gasket. The outer section of the gasket was described in Section 2.2.2. To reiterate, its function is to isolate the fluid plenums and seal the fluids within their plates. The inner section of the gasket encloses the active area to contain the reactant gases within the flow field. Since the inner gasket must cross the channels in the inlet and outlet headers, a plastic bridge was inset underneath the gasket for support. The gas flows from the three tapered sections of the header into the channels at a depth of 4 mm. The gas then travels underneath the inner gasket bridge, where it contracts to a height of 1.2 mm before expanding back to a height of 4 mm. The channels then transition into the flow field in two steps. First, the channel height is reduced to 1 mm for a span of 1.5 mm, at which point the channels become 0.5 mm for the length of the flow field. The channels follow the opposite stepping pattern on the other end of the flow field, where the gas exits into the outlet header. See Figure 2-11 for a cross-section of a single channel along the length of the flow field.
To ensure that there was an even flow distribution among the channels, a similar analysis was performed to that conducted for the coolant plate. A COMSOL laminar flow model was implemented using the 3D geometry of the gas passageway, which was imported from SolidWorks. The design process for the reactant plate flow geometry consisted of several iterations, which were sequentially improved until a satisfactory flow distribution was achieved [46]. Once imported, an appropriate mesh was applied. Using the same method as was used for the coolant plate, the geometry was divided into sections such that the mesh size could be adapted according to the size of the section. The mesh was, once again, refined until the final solution converged. The final mesh consisted of 1,239,168 elements. The final model geometry and an expanded view of the mesh are presented in Figure 2-12. The inlet boundary condition was a mass flow rate and the outlet boundary condition was a constant gauge pressure of 0 Pa.

**Figure 2-11.** Cross-section of reactant flow plate along the length of the flow field

**Figure 2-12.** Model geometry for gas passageways with an expanded view of the mesh

*Note. Axes values are in millimeters*
The inlet boundary condition is based on the consumption rate of oxygen for a specific current draw for fuel cell operation. The inlet air mass flow rate is given by: 

\[ \dot{m}_{a,\text{inlet}} = \frac{\lambda_{O_2} M_a I}{r_{O_2,\text{in}} 4F} \]

For a current density of 1 A/cm² (or current of 8 A) and stoichiometric value of 6 for oxygen, a mass flow rate of 1.711x10⁻³ kg/s of air (or volumetric flow rate of 0.8381 SLPM using a standard dry air density of 1.225 kg/m³) needs to be supplied to the cathode reactant plate. The average velocity for the nine channels, with the 1.588 × 0.5 mm channel cross-section, is 1.955 m/s. This results in a Reynolds number of 101 using a kinematic viscosity for dry air at 15 °C of 1.467x10⁻⁵ m²/s, and the hydraulic diameter of the channel of 0.7605 mm. This proves that the Reynolds number for this case is well below 2300 and therefore can be considered laminar flow.

Surface maps of the resulting velocity profile from the model are shown in Figure 2-13. The inlet header is shown in Figure 2-13(a), the flow field in (b) and the outlet header in (c). Since the headers and flow channels have varying heights (4 and 0.5 mm, respectively), the plotted surface planes in Figure 2-13 are located horizontally along the corresponding midpoint height. The final flow distribution among the nine channels was excellent, deviating a maximum of ±2% from the theoretical average flow rate of 0.09312 SLPM per channel (see Figure 2-14).

Figure 2-13. Surface map of the velocity field for the reactant flow plate for (a) the inlet header, (b) the flow field, and (c) the outlet header.

Note. Axes values are in millimeters.
Figure 2-14. Flow distribution across the nine channels of the reactant flow plate

The final pressure drop across the reactant plate from the model was 134 Pa, which is comparable to the estimated pressure drop solved for using fundamentals of fluid dynamics and the experimental pressure drop (more on this in Section 3.4). Also, the inlet and outlet headers have a low pressure drop (<5 Pa each) in comparison to the flow field, which is favorable for minimizing parasitic pumping losses. See Figure 2-15 for the resulting surface map of the pressure.

Figure 2-15. Pressure distribution across the reactant flow plate

*Note.* Axes values are in millimeters
2.3.2 Quasi in-situ

For the quasi in-situ experiment, the air flow plate and the segmented water plate replace the RFPs between the two coolant plates. The segmented water plate is used as a water chamber on top of the GDL, and the air flow plate is used to supply air along the bottom of the GDL. As mentioned in Section 2.3, the segmented water plate is divided into five equal sections along the length of the flow field. Each section is connected to a water column, which is used to measure the rate of water removal through the GDL for that section. The air flow plate has five pressure taps along the flow field that correspond to the five sections of the water plate. The pressure from each of these taps is used to cap its corresponding water column, in order to balance the pressure from the air side to the water side. A connection network is used to supply water to the water plate, to connect the water columns to the water plate, and to connect the air taps to the top of the water columns. Since the current collectors had protruding tabs that would interfere with the connection network, they were replaced with two rectangular brass plates.

Air flow plate

The air flow plate has identical flow geometry to the RFP, with additional geometry for the pressure taps. Since the flow geometry is the same, this plate will have the same flow characteristics as described for the RFP described in Section 2.3.1. The five pressure taps were cut at the midway point of the water sections, perpendicular to the flow field. See Figure 2-16 for a SolidWorks rendering of the air flow plate and the final fabricated plate. The 1/16” (0.794 mm) wide pressure taps run from the outer channels of the flow field to 3/32” (2.381 mm) diameter blind holes near the edges of the plate. The blind holes are connected to the edges of the plate by 1/16” diameter holes. The inner gasket was modified to create a seal between the blind holes. The
plate was covered in Kapton® tape in order to hydrodynamically isolate the portion of the pressure taps directly adjacent to the channels, as they were otherwise open to each other.

![Figure 2-16. Air flow plate (a) rendered and (b) fabricated](image)

*Segmented water plate*

The segmented water plate has an active area that matches the air flow plate, with walls added to create the water sections. There are four 0.8 mm wide walls equally spaced along the length of the flow field to form the five isolated water sections. The sections have a chamber depth of 2 mm. There are no inlet or outlet headers in this plate. Instead, the same geometry that was used for the pressure taps of the air flow plate was used to connect the water sections to the sides of the plate. That is, passages were cut perpendicular to the flow field at the midway point of the water sections. These 1/16” (0.794 mm) wide passageways run from the outer channels to blind holes near the edges. Once again, the blind holes are connected to the edge of the plate by 1/16” diameter holes. The passageways also continue through the lands of the flow field to connect the
channels within each section. See Figure 2-17 for a SolidWorks rendering of the water plate and the final fabricated plate. In order to seal between the passageways, the inner gasket and Kapton® tape were applied in the same fashion described for the air flow plate.

![Segmented water plate](image)

*Figure 2-17. Segmented water plate (a) rendered and (b) fabricated*

**Connection network**

The connection network consists of four fitting assemblies, as well as a tubing network designed to connect the assemblies. See Figure 2-18 for a schematic of the connection network. The fitting assemblies connect to the sides of each plate in order to extend the pressure taps and water passageways to the exterior of the cell, where they are connected to individual fittings. Each fitting assembly consists of a base plate and a cover plate, which are fabricated out of PMMA (polymethyl methacrylate). The base plate has five channels corresponding to the five water sections, while the cover plate tops the base plate and has five threaded holes for the fittings. The base plate has five 1/16” diameter holes along its mounting edge that align with the holes on the
sides of the air and water plates. These five holes extend to 3/32” diameter blind holes, in a similar manner to that which was used for the pressure taps and water passageways of the test plates. These blind holes are connected to 1/16” wide channels that spread outward to a wider array of 3/16” diameter blind holes. These holes were spaced further apart to provide space for the fittings. These larger blind holes align with the fittings in the cover plate. Kapton® tape was placed over the channels of the base plate to seal between the sections.

Figure 2-18. Schematic of the connection network
The cover plate has 11 countersunk holes for M2 flat head machine screws to pass through and secure the cover to the base plate. Flat O-gaskets (3/16” ID x 3/8” OD x 1/32” (0.794 mm) thick) were hand cut to seal the large blind holes between the base and cover plates. Since the thickness of the O-gaskets would have caused the base and cover plates to flex, which could lead to leakage, the machine screws pass through washers between the plates. The washers were 0.5 mm thick which allowed for compression of the O-gaskets while providing consistent spacing between the base and cover plates. The fittings are thread into the cover plate and have a push-to-connect design for 1/4” OD tubing. They are made out of nickel-coated brass, have 10-32 UNF straight thread, and contain O-rings to seal them against the cover plate. There is a tab with a countersunk hole on either side of each base plate, which allows the fitting assemblies to be properly aligned and screwed into the sides of the test plates. Five 1/16 ID x 3/16 OD O-rings (Size #: 003) are centered about the holes in the edge of the test plate to create a seal between the fitting assembly and test plate.

As mentioned, there are fitting assemblies on both sides of the water plate and air flow plate. For the water plate, the front-side fittings are used to hold the water columns, while the back-side fittings are used to supply water to each of the sections. A 90° ball valve is placed on each of the back-side fittings to plug them after the water is supplied. From each back-side fitting, the water flows through the water passageway and fills the corresponding section chamber. It then flows through the opposite water passageway and fills the corresponding water column attached to the front-side fitting. For the air flow plate, the back-side fittings are used to connect to the pressure taps to the water columns, while the front-side fittings are un-used and therefore plugged. The air pressure is connected from the pressure tap fittings to the tops of the water columns through a series of push-to-connect elbow fittings and tubing. This connection was important to prevent
the pressure along the channels from overcoming the hydrostatic pressure of the water columns, which can cause air flow through the porous GDL and bubbling in the column. This capping system allows any flow rate or back pressure to be applied to the system by ensuring that the sections’ pressures will always be balanced across the GDL.

**Water columns**

The rate of water removal through the GDL for the five sections is measured according to the change in height of the water in each of the five water columns. Since the rate of water removal varies based on several factors (e.g., input air RH and flow rate, GDL sample, flow field geometry), the inner diameter (ID) of the water columns was also varied in order to optimize the drain time. This was important to obtain a similar resolution between tests. Three ID dimensions of standard size tubing were chosen based on estimated rates of water removal. The imperial standard dimensions for the IDs and outer diameters (ODs) are (1) 1/8” ID × 1/4” OD, (2) 3/32” ID × 5/32” OD, and (3) 1/16” ID × 1/8” OD. Notably, the tubes’ IDs decrease in 32nd of an inch increments: 4/32”, 3/32”, and 2/32” (or 3.175, 2.381, and 1.588 mm), respectively. The three sizes of tubing for the water columns were interchangeable by using adapters that were sized according to the ODs. The height from the fittings in the water column fitting assembly to the pressure caps is 120 mm. Since no adapters were needed for the 4/32” ID × 1/4” OD tubing, the heights of the water columns were 120 mm when this sized tubing was used. Since adapters were needed for the smaller-sized tubing, the height of the water columns was decreased to 52.48 mm when using the 3/32” ID tubing, and 56.41 mm when using the 2/32” ID tubing. Clear FEP (fluorinated ethylene propylene) tubing was used for the water columns, as well as for all of the tubing in the connection network.
2.4 Output Air Condenser

The output air condenser was used to evaluate the humidity of the output air. Prior to entering the condenser, liquid water was separated from water vapor in the output air. Specifically, the output air line descended vertically from the underside of the cell into a tube such that any liquid water would run down the tube via gravity into a reservoir placed below the cell. To ensure that the gas did not flow out of the liquid water tube, the reservoir was pre-filled with water and the tube was submerged at least 3 cm. This produced a backpressure of ~300 Pa at the bottom of the tube, which ensured that the humid air flowed into the condenser rather than escaping into the reservoir. A T-valve placed above the reservoir allowed the humid air to pass into the condenser while the liquid water dripped out below.

The condenser itself is a home-made coaxial tube-in-tube heat exchanger. A copper tube (3/8” OD × 5/16” ID) was placed concentrically within a larger PVC (polyvinyl chloride) tube (13/16” OD × 9/16” ID) that was capped at both ends. The copper tube runs through the two capped ends of the PVC tube. The humid air from the cell flows through the inner copper tube, while a cocurrent cold water flow passes through the annulus surrounding the copper tube. The condenser was 2 feet long and set at a 50° angle (from horizontal), so that the condensate on the inside of the copper tube drips downward. The upper end of the copper tube is attached to the output air line, while the lower end extends out of the PVC tube where the condensate drips into a second reservoir. The cold water is supplied to the upper end of the condenser at approximately 10°C and exits at the lower end through fittings in the side of the PVC tube. To cool the water, a submersible pump circulates the water through 60 feet of copper tubing, which is coiled inside a small refrigerator. The water flowed through the system at approximately 264 mL/min.
Both reservoirs were placed on scales to measure the rate at which water was collected. A layer of mineral oil was placed on top of the water in each reservoir to prevent evaporation. Since the air exhausted from the condenser is in a saturated condition (i.e., 100% RH), it will still contain water vapor. Hence, the temperature of the condenser exhaust air was measured by a thermocouple inserted in the copper tube at the lower end of the condenser. During testing, the outlet air remained consistently below 15°C. The saturation pressure at the corresponding air temperature was used to determine the amount of water vapor in the air leaving the condenser. The final water content of the output air was found by summing the rates of the collected liquid water and the rate of water vapor leaving the condenser. See Figure 2-19 for a photo of the condenser system.

*Figure 2-19. Photo of the condenser system*
Compact Salter® electronic scales (Model: 1250BKEF) were used to weigh the collected water. Since the scales were originally digital with no data acquisition output, the electronics were modified to provide an analog voltage output. To achieve this, the digital circuitry of each scale was removed and the scales’ sensors were connected to supplementary external circuitry. The sensor in each scale is a Wheatstone bridge, which converts a voltage input into an output voltage signal proportional to the weight on the scale. The output voltage signal was amplified using a Texas Instruments LM741 CN operational amplifier (op-amp) in order to obtain a measurable voltage signal. See Figure 2-20 for a circuit diagram of the electrical system.

![Circuit diagram of the electric system](image)

Figure 2-20. Circuit diagram of the electric system

The E+ and E- nodes of the Wheatstone bridge are supplied with 3 V from two AAA batteries. The V+ and V- nodes of the op-amp are supplied with 18 V from two 9 V batteries. The V+ node is supplied with +9 V and the V- node is supplied with -9 V by connecting the anode of one battery to the cathode of the other battery. All of the batteries were recharged between tests. The S+ and S- nodes of the Wheatstone bridge are the sense leads from the scale. S+ is the output from the Wheatstone bridge and is connected to the op-amp for amplification. The S- node is connected to the ground node. The op-amp is set in a non-inverting configuration. The voltage gain from V_in to V_out of the op-amp is calculated as \( G = 1 + \left( \frac{R_2}{R_1} \right) \). The resistance of R_1 and R_2 were 1 k\( \Omega \) and 1.51 M\( \Omega \), respectively. Therefore, the voltage gain is G=1511. The output voltage
signal, $V_{out}$, is recorded by a PASCO ScienceWorkshop® 750 Interface at 1 Hz, which is connected to the computer for data acquisition.

The scales could weigh a maximum of 500 g. Therefore, 500 mL plastic containers were used as the two reservoirs. A glass slide was fixed to the bottom of each container to avoid off-center weighing. The scales were calibrated using a 125-point calibration method. Fastener nuts, with an average weight of 3.5056 g (SD=0.0820 g), were used as standard weights and placed on the scale incrementally. The group of nuts weighed 438.2 g and the reservoir weighed 20.7 g, which together approximated the weighing range of the instrument. The corresponding voltage output signals were recorded and plotted against the weight on the scale. This calibration curve is presented in Figure 2-21. As can be seen, a linear fit was obtained and the final sensitivity was consistent at 96.841 g/V. The signal-to-noise ratio of the electrical system limited the resolution of the recorded voltage to 0.010 V. Therefore, the accuracy of the scales was approximately ±1 g.

\[ W = 96.841*V - 82.892 \]
\[ R^2 = 1.000 \]

*Figure 2-21. Calibration curve for the scales*
CHAPTER 3: EXPERIMENTAL METHODS

This chapter provides specifications of the materials used. It also defines and tabulates the input test conditions. It then describes important aspects of the test cell assembly, followed by a description of the test procedure for each type of experiment. Finally, it explains how the data from each type of experiment were collected and analyzed.

3.1 Materials

The reactant, air, water, and coolant plates were machined out of 1/4” (6.35 mm) Graphtek LLC Impervious Bipolar Graphite Plate. This material has a high thermal conductivity and low electrical resistance, good machinability and excellent chemical resistance. The gasket material used was a 3/32” EPDM (ethylene-propylene-dienemonomer) rubber sheet, which has a Durometer hardness of 60A. It can be used up to a temperature of 110°C and is water and chemically resistant. The connection fitting assemblies’ plates were machined out of 6.35 mm Acrylite® PMMA. Swagelok fittings (316SS) are attached to the manifold to connect the fluids lines. All gases were from Air Liquide’s ALPHAGAZ 1 product line. The purity of the nitrogen and hydrogen are rated as >99.999%, and the oxygen concentration in the air is rated as 20-22%.

For the in-situ experiment, a 7-layer MEA was used, consisting of a 3-layer CCM and two dual-layer GDLs. The 3-layer CCM (Yangtze XL-3BP-318) used Nafion XL as the PEM and has a catalyst loading of 0.4 mg/cm² of 40% Pt/C on the air side (cathode) and 0.2 mg/cm² of 40% Pt/C on the hydrogen side (anode). The total thickness of the CCM is 74 ± 5 μm. The anode GDL was AvCarb GDS3215 and was used as a commercial baseline. This 200 μm dual layer gas diffusion system has a teflonated AvCarb EP40 carbon fiber substrate coated with an MPL. The cathode GDL (also used for the quasi in-situ experiment) has an AvCarb EP40 carbon fiber substrate with a 12 wt.% PTFE content. It is coated with a carbon black MPL which has a PTFE
content of 18 wt.% and an areal weight loading of 15 ± 2 g/m². The total thickness of this GDL is 190 μm. This GDL was provided by Ballard Power Systems and its ex-situ properties have been characterized in other studies [47, 48, 49]. Figure 3-1 shows a scanning electron microscope (SEM) image of the carbon fiber substrate (left) and the MPL (right), for the cathode GDL.

![Figure 3-1. SEM images of the cathode GDL (left) and MPL (right)](image)

3.2 Test Conditions

The experimental test conditions for both types of experiments are listed in Table 3-1. The cathode air conditions consisted of two flow rates, low and high, and four relative humidity conditions, ranging from dry to oversaturated. The hydrogen was kept fully humidified and the cell temperature was held constant at 70°C. As previously mentioned, the quasi in-situ experiment used the same air conditions as the cathode air of the in-situ experiment. The input flow rates for the air and hydrogen are found using Equations 3.1 and 3.2, respectively.

\[
\dot{m}_{a,\text{inlet}} = \frac{\lambda_{O_2}}{r_{O_2,\text{in}}} \frac{M_a I}{4F} \tag{3.1}
\]

\[
\dot{m}_{H_2,\text{inlet}} = \frac{\lambda_{H_2}}{2F} \frac{M_{H_2} I}{2F} \tag{3.2}
\]
The flow rates chosen for the air were found using an oxygen stoichiometry ($\lambda_{O_2}$) of 3 at 1 A/cm$^2$ (i.e., 8 A) for the low flow rate and 6 at 1 A/cm$^2$ for the high flow rate condition. The oxygen volume fraction ($r_{O_2}$) at the inlet air was 0.21. A standard dry air density of 1.225 kg/m$^3$ was used to convert the mass flow rate into a volumetric flow rate in standard liters per minute (SLPM). The flow rate for the hydrogen was found based on a hydrogen stoichiometry ($\lambda_{H_2}$) of 6 at 1 A/cm$^2$ and a standard hydrogen density of 0.0853 kg/m$^3$. The inlet air RH levels chosen were 35%, 65%, 95%, and 125%. The corresponding dew point temperatures are listed in Table 3-1. The air RH value exceeds 100% when the air is oversaturated and liquid water is present. The inlet anode RH was 100%. The reactant gas temperatures were both 70°C (equal to the cell temperature). The input test conditions are denoted as ‘air inlet RH-oxygen stoichiometry’. For example, for a 65% air inlet RH and an oxygen stoichiometry of 6 at 1 A/cm$^2$, the condition is referred to as 65-6.

*Table 3-1. Input test conditions*

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell temperature</td>
<td>70°C</td>
</tr>
<tr>
<td>Hydrogen flow rate</td>
<td>$\lambda_{H_2} = 6$ at 1 A/cm$^2$</td>
</tr>
<tr>
<td></td>
<td>0.352 SLPM</td>
</tr>
<tr>
<td>Hydrogen gas temperature</td>
<td>70°C</td>
</tr>
<tr>
<td>Hydrogen relative humidity</td>
<td>100%</td>
</tr>
<tr>
<td>Corresponding hydrogen dew point temperature</td>
<td>70°C</td>
</tr>
<tr>
<td>Air flow rate</td>
<td>Low flow rate</td>
</tr>
<tr>
<td></td>
<td>$\lambda_{O_2} = 3$ at 1 A/cm$^2$</td>
</tr>
<tr>
<td></td>
<td>0.419 SLPM</td>
</tr>
<tr>
<td>Air gas temperature</td>
<td>70°C</td>
</tr>
<tr>
<td>Air relative humidity</td>
<td>35%</td>
</tr>
<tr>
<td>Corresponding air dew point temperature</td>
<td>47.41°C</td>
</tr>
<tr>
<td></td>
<td>65%</td>
</tr>
<tr>
<td></td>
<td>95%</td>
</tr>
<tr>
<td></td>
<td>125%</td>
</tr>
<tr>
<td></td>
<td>60.33°C</td>
</tr>
<tr>
<td></td>
<td>68.73°C</td>
</tr>
<tr>
<td></td>
<td>75.24°C</td>
</tr>
</tbody>
</table>
3.3 Cell Assembly

Having defined each of the components of the test cell and test plates in Chapter 2, see Figure 3-2 for a photo of the disassembled system for both the in-situ (right) and quasi in-situ (left) experiments. The following procedure was used to assemble the cell for both types of experiments:

1. The current collectors, or brass plates, are inset into the piston top and manifold backing plate.
2. One coolant plate is centered on top of the piston backing plate (the piston top) with the channels facing upwards.
3. The anode RFP (i.e., reactant flow plate), or segmented water plate, is placed on top of the coolant plate with the channels facing upwards.
4. The MEA, or GDL, is centered about the active area.
5. The cathode RFP, or air flow plate, is placed on top of the anode RFP, or segmented water plate, with the channels facing downwards.
6. The other coolant plate is placed on top of the cathode RFP, or air flow plate, with the channels facing downwards.
7. The manifold backing plate is placed on top of the coolant and test plates, with the inlet and outlet manifolds facing upwards.
8. The six tie bolts are secured in a multiple pass tightening sequence to avoid an uneven preload across the plates.
9. Nitrogen is supplied to the piston at 60 psig to compress the cell.
10. The cell is flipped 180° and placed into a hanging apparatus to suspend the test cell within the test station, and is leveled by adjusting turnbuckles. This orients the cell horizontally with the anode, or the water side, above the cathode, or the air side.
Figure 3-2. Disassembled test cell and test plates for in-situ (right) and quasi in-situ (left)
See Figure 3-3 for a photo of the assembled test cell containing the in-situ test plates (left) and the quasi in-situ plates with the connection assembly (right). Aspects of the cell assembly that differ between the in-situ and quasi in-situ experiments are described in the following subsections.

### 3.3.1 In-situ

For the in-situ experiment, a CCM is placed between two GDLs to form the MEA, which is sandwiched between the reactant plates. Two spacing layers are positioned between the anode and cathode to electrically insulate the electrodes and physically isolate the reactant plates from each other. Each layer covers the entire surface of the reactant plate except for the inlet and outlet holes, and the active area where the MEA sits. The spacing layers also assist in achieving the appropriate compression of the GDLs. Since the spacing layers are incompressible in comparison to the GDLs, they act as dead-stops, such that the lands of the flow fields compress into each GDL a fixed amount. This method ensures that excessive piston pressure does not crush the GDLs. Each spacing layer is 150 μm thick and each GDL is ~200 μm thick. Therefore, each GDL is compressed 25% underneath the lands.

### 3.3.2 Quasi in-situ

For the quasi in-situ experiment, a single GDL is situated between the segmented water plate and air flow plate. Accordingly, the spacing technique was altered in order to achieve the same 25% compression of the GDL. The Kapton® films that cover the quasi in-situ test plates, described in Section 2.3.2, also function as the spacing layers for this experiment. Since each Kapton® layer is 75 μm, the total spacing thickness is 150 μm, which is equivalent to one in-situ spacing layer. Therefore, the single GDL achieves the same compression. The GDL is placed over the entire active area of the water plate with the MPL side facing down. The edges of the GDL protrude past the active area and rest in a 75 μm ledge inset around the active area of the water and
air plates, such that the GDL achieves contact with the lands. The GDL ledge is bordered in Teflon tape, which acts as a hydrophobic barrier to create a water seal between the air and water sides.

Prior to assembly, the five sections of the water plate are filled with water, so that all of the walls are coated. This is to ensure that water fills the entire water chamber during the initial purge without forming bubbles, which can occur within a dry assembly as droplet pinning can prevent water from entering small sections. To attach the fitting assemblies and water columns, the cell is placed in an intermediate assembly jig. First, the O-rings are aligned with the five holes on either side of each test plate; the surface tension of water is used to initially hold them on. Then, the fitting assemblies are fastened to the plates and a thin supporting beam is placed underneath each assembly unit to avoid torqueing. The water columns are attached to the front-side fittings and the connection network tubing is constructed around the cell in order to connect the pressure taps to the tops of the water columns.

There were several areas vulnerable to potential leakage of water in the quasi in-situ setup. The challenges involved in sealing pressurized water on one side of a GDL with an adjacent air side have been discussed in other studies [26, 50]. Three main criteria were evaluated before beginning the quasi in-situ test:

1. No leaking of water between the water and air side (solved by Teflon tape border)
2. No leaking between the water columns (solved by gaskets, O-rings, and Kapton®)
3. Compression of GDL and contact between graphite plates (solved with the 75 μm ledge inset around the active area of the water and air plates)

Criteria 1 and 2 were confirmed when the water columns could be filled with no change in height of the water in the columns overnight (18+ hrs; see Figure 3-4). Numerous attempts and iterations were required before these criteria were met. Criterion 3 was confirmed with a conductivity test.
Figure 3-3. Assembled test cell for in-situ experiment (left) and quasi in-situ experiment (right)

Figure 3-4. Water columns immediately after being filled (left) and 18 hours later (right)
3.4 Cell Validation and Condenser Calibration

Before experimental testing, the system was taken through a validation procedure. The coolant and reactant flow plates were assembled in the test cell. A single spacing layer was placed between the RFPs that covered the entire reactant plate surface, including the active area, except for the inlet and outlet holes. To ensure the gasket system was correctly sealed, the outlet was dead-ended and the system was pressurized at 10 psig to check for leakage. A manual pressure gauge at the inlet showed no drop and, hence, no leakage from the gaskets or fittings. The RFP was then tested for pressure drop, using 20°C dry air. Figure 3-5 shows the experimental pressure drop versus the flow rate obtained for the RFP. From this curve, the pressure drop at 0.838 SLPM is 131 Pa. This agrees well with the pressure drop of 134 Pa found at the same flow rate from the COMSOL model (noted in Section 2.3.1). Using this cell validation setup, the condenser was calibrated by flowing humid air through the system and comparing the water vapor entering the system to the amount of water collected by the condenser (i.e., the sum of liquid water caught by the trap, condensate from the condenser, and water vapor in the condenser exhaust air). A cell and air temperature of 70°C and an air flow rate of 0.838 SLPM were used. The air RH was stepped from 35%-140% at increments of 15%. As evident in the calibration results in Figure 3-6, the input and output rates are all statistically equivalent, proving that the condenser system works well.

![Figure 3-5. Pressure versus flow curve for air in the reactant flow plate](image-url)
3.5 Test Procedure and Data Analysis

This section describes the testing procedures, as well as the techniques used for collecting and analyzing the data for the in-situ and quasi in-situ experiments.

3.5.1 In-situ

For the in-situ testing, the cell was brought to its set-point temperatures with co-flowing, fully humidified reactants. The cell was then put through a preliminary ten-hour cycle to hydrate the PEM. The ten-hour cycle consists of holding the cell at 0.6, 0.4, and 0.2 V for two hours each, then performing a two-hour voltage scan, and then holding the cell at 0.6 V for another two hours. Between test conditions, three hours were provided in order for the dew point temperature and cell to reach a steady state. Two techniques were used to characterize the cell performance across the set of eight input test conditions. The first was the common polarization curve. The open-circuit voltage was recorded for one minute. Then, a voltage staircase was performed and the current was recorded at 1 Hz (i.e., chronoamperometry). The voltage was stepped from 0.85 V to 0.05 V, with a 50 mV step height and a 10 minute step time. The last 7 minutes of each step (420 data points) was analyzed to find the range (minimum and maximum), median, and 25% and 75% quartiles of
the recorded current. The current was normalized by the active area of 8 cm$^2$, and the output power density was found using the product of voltage and current density.

Once the polarization curve was complete, the second technique that was used to characterize the performance was holding the cell at a constant current of 1 A/cm$^2$ for 2.5 hours, while recording the voltage at 1 Hz (i.e., chronopotentiometry). The current density of 1 A/cm$^2$ was selected because preliminary tests identified this point as a threshold for the presence of mass transport losses for the majority of the input conditions. Also, using a constant current facilitates the evaluation of the consumption rate of the reactants and production rate of water. The last 2 hours of the recorded voltage was analyzed to obtain the range (minimum and maximum), median, and 25% and 75% quartiles. A factorial analysis of variance (ANOVA) was computed on the output power densities obtained from this chronopotentiometric testing in order to examine the main effects and interaction effect of the air flow rate and RH on cell performance [51, 52]. This procedure tests whether the power density outputs statistically differ across input conditions.

The relative humidity levels in the output air and hydrogen were found using the condenser data during the constant current testing. First, the rates of water from the water trap, output condensate, and condenser exhaust air were summed. Next, the total rate of the collected water, along with the known water production rate and the reactants’ inlet and outlet flow rates and RH levels, were used to perform a water balance. The system of equations used to perform this analysis is explained below, starting with the water balance described in Equation 3.3.

$$
(m_a \omega_a + m_{H_2} \omega_{H_2})_{inlet} + m_{production} = (m_a \omega_a + m_{H_2} \omega_{H_2})_{outlet}
$$

(3.3)

In Equation 3.3, the inlet air and hydrogen mass flow rates ($m_a$ and $m_{H_2}$)$_{inlet}$ are found using Equation 3.1 and Equation 3.2, respectively. Since oxygen and hydrogen are being consumed in
the reaction, the outlet air and hydrogen mass flow rates \( \left( \dot{m}_a \text{ and } \dot{m}_{H_2} \right)_{\text{outlet}} \) are found using Equation 3.4 and Equation 3.5, respectively. The amount of water production is shown in Equation 3.6. The amount of water collected by the condenser is equal to the water content in the output air, as shown in Equation 3.7. The humidity ratio of the air and hydrogen are found using Equation 3.8 and Equation 3.9, respectively.

\[
\dot{m}_{a,\text{outlet}} = \left( \frac{\lambda_{O_2} - 1}{M_{O_2}} \lambda_{O_2} \frac{(1-r_{O_2,\text{in}})}{r_{O_2,\text{in}}} M_{N_2} \right) \frac{I}{4F} \quad (3.4)
\]

\[
\dot{m}_{H_2,\text{outlet}} = (\lambda_{H_2} - 1) \frac{M_{H_2} I}{2F} \quad (3.5)
\]

\[\dot{m}_{\text{production}} = \frac{M_{H_2} I}{2F} \quad (3.6)\]

\[\dot{m}_{\text{collected}} = (\dot{m}_a \omega_a)_{\text{outlet}} \quad (3.7)\]

\[\omega_a = \frac{0.6219 \phi_a p_s}{(P - \phi_a p_s)} \quad (3.8)\]

\[\omega_{H_2} = \frac{9 \phi_{H_2} p_s}{(P - \phi_{H_2} p_s)} \quad (3.9)\]

From this system of equations, the RH of the outlet air can be found by combining Equations 3.4, 3.7, and 3.8, as presented in Equation 3.10. The RH of the outlet hydrogen can be found by combining Equations 3.1-3.9, as presented in Equation 3.11.

\[\omega_{a,\text{outlet}} = \frac{\dot{m}_{\text{collected}}}{\dot{m}_{a,\text{outlet}}} \rightarrow \phi_{a,\text{outlet}} = \frac{P}{p_s \left( 1 + \frac{0.6219}{\omega_{a,\text{outlet}}} \right)} \quad (3.10)\]

\[\omega_{H_2,\text{outlet}} = \frac{(\dot{m}_a \omega_a + \dot{m}_{H_2} \omega_{H_2})_{\text{outlet}} + \dot{m}_{\text{production}} - \dot{m}_{\text{collected}}}{\dot{m}_{H_2,\text{outlet}}} \rightarrow \phi_{H_2,\text{outlet}} = \frac{P}{p_s \left( 1 + \frac{9}{\omega_{H_2,\text{outlet}}} \right)} \quad (3.11)\]
3.5.2 Quasi in-situ

For the quasi in-situ setup, the air in the five water sections was purged as de-ionized (DI) water was input to the section chambers. Once the chambers were purged and the water columns were filled, the cell temperature and the gas and dew-point temperatures of the air were brought to their set-points. The two air flow rates (low and high) were run at one RH per day, and three repeat runs were conducted for each test condition. One repeat run consisted of all of the water draining from the first water column and the columns were refilled for each additional run. The water columns were recorded during testing so that the images could be analyzed to find the rate of water removed from each column.

A GoPro (Hero3-Silver Edition) camera was used to perform time-lapse imaging in order to capture the rate of water removal for the water columns. The camera was set to take photos every 10 seconds at an 11 megapixel resolution (3680 x 2760 pixels). The camera was rotated 90° such that portrait-oriented images were captured. This vertically-oriented wide field of view was the most suitable orientation for capturing the height of the water columns at the highest pixel resolution. The GoPro was mounted on a flexible mounting arm, which had a stage attached to one end. The stage was manually adjusted prior to conducting each test to ensure that it was level. During testing, the GoPro was connected to a charging plug. A black velvet sheet was attached with Velcro to the perimeter of the test station to block out surrounding light during testing. Two strips of LED lights illuminated the water columns, and the light was diffused by covering each LED strip with a Kimwipe® in order to reduce glare. A white piece of paper was placed behind the water columns to provide a background that would give good contrast between each side of the water/air interface in the columns. See Figure 3-7 for a picture of the recording setup.
Since the images that were obtained had GoPro’s iconic ‘fisheye’ distortion and were rotated 90°, they had to be corrected. Subsequently, the water removal rates for each of the five columns had to be extracted from the pixelated image data. A pair of MATLAB programs were created to accomplish these tasks. The first program corrects the raw images for orientation and distortion, and then combines the corrected images into a video using specified time increments. The second program reads in the video that was created by the previous program and allows the user to manually extract the rate of water removal for each of the five columns, using a point-and-click method. The selected pixel points are then translated into centimeters using a calibrated pixel density, which are then converted into a volumetric flowrate based on the inner diameter of the water column. These two programs will now be described in greater detail.

The first MATLAB program was used to rotate each image 90°, so that the water columns appeared upright. Subsequently, the images were corrected for barrel (i.e., ‘fisheye’) aberrations, which occur when the image magnification decreases radially from the optical axis. This correction was achieved using a downloaded LENSDISTORT function (de Vries, 2012), which was retrieved.
from MATLAB’s open-source File Exchange platform [53]. This program requires the user to define a *k-factor* (i.e., distortion parameter), which determines the extent to which the image is corrected. To find the optimal correction factor for the images, several distortion parameters were applied to a single test image and the resulting set of trial images were visually analyzed to determine which *k*-factor made the water columns in the image appear straightest. Figure 3-8 shows an example set of images including an original rotated image, a final corrected image, and an over-corrected image. Based on this analysis, a *k*-factor of -0.30 was selected and applied to all of the subsequent images. The final corrected images became single frames which were combined into a video file.

![Figure 3-8](image.png)

*Figure 3-8. Example set of trial images including (a) an original image rotated 90°, (b) a final corrected image \([k = -0.30]\), and (c) an over-corrected image \([k = -0.40]\)*

Since the duration of each test varied according to the test’s input air conditions and ID of the water columns, the total number of images obtained for each test also varied. To account for this, the program selected images at specified time increments that were proportional to the test duration. The specified time increments were determined based on the number of images required...
before there was a visually detectable change in the water height. For example, for a test with inputs of 35% RH and high flow rate as well as an inner tube diameter of 3/32\textquotedbl", every third image was selected. Since images were recorded every 10 seconds, each frame in the resulting video would represent a 30-second interval. In contrast, for a test with inputs of 65% RH and low flow rate with the same inner tube diameter of 3/32\textquotedbl", the water was removed more slowly and, therefore, every sixth image was selected. Each frame in this video would therefore represent a 60-second interval. This procedure produced videos that were consistent in total number of frames, which was important in order to obtain an equivalent number of points in the height extraction process.

The second MATLAB program was used to extract the rate at which water in each column was removed. To do this, the program loaded a video created by the first program and each video frame was cropped into five sections, one for each water column. Next, the user was prompted to manually select the height of the water in each column frame-by-frame (i.e., at progressing time intervals); each selection produced a pixel value (see Figure 3-9). The normalized pixel value in each frame was converted into a metric height by applying a calibrated pixel density. This pixel density was found by using the same point-and-click method to determine the pixel height of a known dimension in a specific image. In order to obtain an accurate calibration, the known dimension had to be located on the same plane as the columns (i.e., at the same distance away from the camera). Hence, the lengths of the columns themselves served this purpose well. An example of this calibration technique is provided in Figure 3-9. In this example, the known column height is 5.248 cm and the pixel height is 1530 pixels, resulting in a pixel density of 0.00343 cm/pixel.

Using the pixel results for the three repeat runs the pixel density was applied to find the change in height of a water column as a function of time. The mean rate and 95% confidence interval were found using Excel’s TREND function and are shown in Figure 3-10. As can be seen,
good repeatability was shown between the three runs. To evaluate test-retest reliability and inter-rater reliability of the MATLAB extraction program, two extraction trials of a single column were performed by the author on two different occasions and a separate trained user completed a third trial. These trials demonstrated acceptable reliability and are compared in Table 3-2.

![Image](image.png)

**Figure 3-9.** Example to find pixel density and change in height of the water column

*Note.* The final pixel density for this example is 0.00343 cm/pixel

The speed at which water was removed was then converted to a volumetric flow rate using the ID of the water column. The volumetric flow rate obtained for each run was converted into a mass flow rate using the density of water at 20°C of 998 kg/m³. Finally, the rates of water removal from the five water columns were transferred into a concentration profile using Equation 3.12 and, subsequently, Equation 3.13. This profile demonstrates the increase of air RH along the length of the flow field due to the addition of water diffusing through the GDL.
\[
\omega_{a,i+1} = \omega_{a,i} + \frac{\dot{m}_{p,i}}{m_a} \\
\phi_{a,i+1} = \frac{P}{p_s \left(1 + \frac{0.6219}{\omega_{a,i+1}}\right)}
\] (3.12) (3.13)

Figure 3-10. Height of the water column as a function of time

Table 3-2. Results from test-retest and inter-rater reliability checks

<table>
<thead>
<tr>
<th>User (trial number)</th>
<th>Rate [cm/min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>R.P. (1)</td>
<td>0.3318 ± 0.0088</td>
</tr>
<tr>
<td>R.P. (2)</td>
<td>0.3348 ± 0.0161</td>
</tr>
<tr>
<td>M.J. (1)</td>
<td>0.3307 ± 0.0098</td>
</tr>
</tbody>
</table>

Note. Means are reported with 95% confidence intervals
CHAPTER 4: GOVERNING EQUATIONS FOR INTERNAL FLOW

This chapter will document the governing equations for internal flow in a rectangular channel. It will serve as the basis for the analytic model that is used for extracting the effective water vapor diffusion coefficient of the GDL from the experimental data, presented in Chapter 5. Hydrodynamic considerations are outlined in Section 4.1, correlations for heat transfer presented in Section 4.2, and the heat and mass transfer analogy discussed in Section 4.3. The elementary equations for humid air properties are reviewed in Appendix A.

4.1 Hydrodynamic Considerations

The Reynolds number (Equation 4.1) represents the ratio of the inertia forces to the viscous forces. Its magnitude can be used to determine the flow regime of the fluid and also to evaluate hydrodynamic considerations for flow.

\[
Re = \frac{\bar{u}L}{v}
\]  

(4.1)

The characteristic length scale, \(L\), is dependent on the flow case at hand (e.g., internal or external flow). For the case of internal flow in a circular pipe, the diameter of the pipe is used for the characteristic length scale. For a rectangular channel the hydraulic diameter is commonly used as the characteristic length, defined by Equation 4.2.

\[
L = d_h = \frac{4A_y}{P} = \frac{2H_{GC}W_{GC}}{H_{GC} + W_{GC}}
\]  

(4.2)

The Reynolds number is given in Equation 4.3 for internal flow based on the hydraulic diameter.

\[
Re_D = \frac{\bar{u}d_h}{v} = \frac{\dot{m}d_h}{\mu A_y}
\]  

(4.3)
The cross-sectional flow area is given in Equation 4.4. The Reynolds number must fall below 2300 to remain in the laminar flow regime; \( Re_d < 2300 \) (for laminar flow). It will be shown below that the flow always remains in the laminar regime for the conditions in this study.

\[
A_c = H \frac{W}{\alpha_c}
\]  

(4.4)

The average velocity for a cross section of internal flow is shown in Equation 4.5.

\[
\bar{u} = \frac{\dot{m}}{\rho A_c}
\]  

(4.5)

Using the energy equation for fluid flow (Equation 4.6), the pressure drop of a horizontal channel may be derived as Equation 4.7, as shown in Wilcox (2005) [54].

\[
\frac{P_i}{\rho g} + \frac{\bar{u}_i^2}{2g} = \frac{P_e}{\rho g} + \frac{\bar{u}_e^2}{2g} + h_L
\]  

(4.6)

\[
\Delta P = (P_i - P_e) = \frac{\rho}{2} (\bar{u}_e^2 - \bar{u}_i^2) + \rho g h_L
\]  

(4.7)

The major head loss in a straight channel can be found using Equation 4.8, where \( f_d \) is the Darcy friction factor [54]. The friction factor represents the magnitude of the surface shear stress due to the velocity gradient from the wall to the fluid flow, and it is used to evaluating the surface frictional drag forces that cause the pressure to drop [25].

\[
h_L = f_d \frac{\bar{u}_i^2}{2g} \frac{L}{d_h}
\]  

(4.8)

The Fanning friction factor, \( f_f \), is another dimensionless parameter that may be used to evaluate the head loss [54]. The Darcy friction factor is defined as four times the Fanning friction factor, and they are used interchangeably based on the relationship given in Equation 4.9.
\[ f_d = 4f_f \] (4.9)

For fully developed laminar flow in a channel, the product of the friction factor and the Reynolds number is independent of channel length [3, 25, 54-56]. For a circular channel, its constant value can be derived as \( f_f Re_p = 64 \) [3, 25, 54-56]. For a rectangular channel, its value is dependent on the aspect ratio of the channel. In this study, the aspect ratio is defined as the ratio of the height (depth) of the channel to the width of the channel, as given in Equation 4.10.

\[ \varepsilon = \frac{H_{GC}}{W_{GC}} = \frac{b}{a} \] (4.10)

Conventional fuel cell channels are commonly designed with approximately 1 mm squared channels (leading to an aspect ratio of 1). For this study, the height of the channel is 0.5 mm and the width of the channel is 1.588 mm (leading to an aspect ratio of 0.3149).

Several correlations have been reported in literature for the friction factor-Reynolds number product for fully developed laminar flow in a rectangular channel [3, 25, 54-58]. Examples are given below and their values listed in Table 4-1 for an aspect ratio of 1 and 0.3149.

Shah and London (1978, p. 199) [56] give the correlation shown in Equation 4.11.

\[ f_f Re_p = 24 \left[ 1 - 1.3553\varepsilon + 1.9467\varepsilon^2 - 1.7012\varepsilon^3 + 0.9564\varepsilon^4 - 0.2537\varepsilon^5 \right] \] (4.11)

Kays and Crawford (1993, p. 80) [55] graphically show the Fanning friction factor-Reynolds product as a function of aspect ratio; the values found in Table 4-1 where visually depicted. Bergman, Lavine, Incropera, and Dewitt (2011, p. 553) [25] tabulate the values for various aspect ratios; the value is found through interpolation for the aspect ratio of 0.3149. Barbir (2005, p. 173) [3] reports the relationship given in Equation 4.12.
\[ f_d Re = 55 + 41.5 \exp(-3.4\varepsilon) \]  

(4.12)

Table 4-1. Darcy friction factor-Reynolds number product for fully developed laminar flow in rectangular channels with varying aspect ratios

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>( \varepsilon = 1 )</td>
<td>Eq. 4.11</td>
<td>Graphically</td>
<td>Tabulated</td>
<td>Eq. 4.12</td>
<td>Eq. 4.15</td>
<td>Eq. 4.16*</td>
</tr>
<tr>
<td>( \varepsilon = 0.3149 )</td>
<td>56.918</td>
<td>56.800</td>
<td>57.000</td>
<td>56.385</td>
<td>56.528</td>
<td>56.528</td>
</tr>
<tr>
<td></td>
<td>69.290</td>
<td>69.800</td>
<td>69.704</td>
<td>69.227</td>
<td>69.196</td>
<td>81.072</td>
</tr>
</tbody>
</table>

*Characteristic length scale based on the square root of cross-sectional flow area

Muzychka and Yavanovich (2002) [58] proposed a model for the laminar flow friction factor in non-circular ducts for fully developed flow, and successively a correlation for hydrodynamically developing flow. The authors recommend that the characteristic length scale should be based on the square root of the cross-sectional flow area, instead of the traditionally used hydraulic diameter. Using this characteristic length scale, shown in Equation 4.13, the Reynolds number (based on the square root of the cross-sectional flow area) is presented by Equation 4.14.

\[ L = \sqrt{A_c} \]  

(4.13)

\[ Re_{c\varepsilon} = \frac{u\sqrt{A_c}}{v} = \frac{\dot{m}}{\mu\sqrt{A_c}} \]  

(4.14)

They [58] derive expressions for the friction factor-Reynolds number product using these two characteristic length scales; the first based on the traditionally used hydraulic diameter (Equation 4.15 [sic]) and the second was based on using their suggested square root of the cross-sectional flow area (Equation 4.16). The validity of the model is proven in their work and will be discussed more below [58, 59].
\[
f_f Re_D = \frac{24}{(1 + \varepsilon)^2 \left[ 1 - \frac{192 \varepsilon}{\pi^5} \tanh \left( \frac{\pi}{2 \varepsilon} \right) \right]}
\]

(4.15)

\[
f_f Re_{\varepsilon} = \frac{12}{\sqrt{\varepsilon} (1 + \varepsilon) \left[ 1 - \frac{192 \varepsilon}{\pi^5} \tanh \left( \frac{\pi}{2 \varepsilon} \right) \right]}
\]

(4.16)

The friction factor-Reynolds product found in Table 4-1 using Equation 4.16 for an aspect ratio of 0.3149 may seem inflated compared to the other values found. This is because its value is based on using the square root of the cross sectional flow area as the characteristic length scale for calculating the Reynolds number. One can simply divide the friction factor-Reynolds product by the Reynolds number at hand and find that the friction factor for the same geometry and flow conditions will remain constant, thus proving that the proposed model is valid. The friction factor-Reynold product is not inflated for an aspect ratio of 1, since the hydraulic diameter will always equal the square root of the cross-sectional flow area for square channels (same value for the characteristic length scale).

For example, for this study’s cross sectional channel geometry of 0.5 × 1.588 mm (\(\varepsilon = 0.3149\)), the hydraulic diameter (Equation 4.2) is 0.7605 mm, and the square root of the cross-sectional flow area (Equation 4.13) is 0.8911 mm. Take the case of humid air flowing through this single channel at 70 °C and 100% RH, with a dry air mass flow rate of 1.8938x10^{-6} kg/s. The mixture (dry air and water vapor) mass flow rate is 2.4173x10^{-6} kg/s and the mixture dynamic viscosity is 17.3979x10^{-6} Pa·s (from Table A-3). The Reynolds number for this case based on the hydraulic diameter (Equation 4.3) is 133.1, and based on the square root of the cross-sectional flow area (Equation 4.14) is 155.9. Dividing these Reynolds number by the respective friction factor-Reynolds product from Table 4-1 yields the constant Darcy friction factor of 0.52.
The Reynolds numbers presented above is a worst case scenario that will produce the highest Reynolds number possible for the conditions in this study. Since it falls well below 2300, it proves that the flow will remain laminar.

Muzychka and Yavanovich have provided detailed descriptions of the validity of this method and the improvements that this model contributes in their publications [58, 59]. In short, through dimensional analysis the authors prove that the characteristic length scale based of the square root of the cross-sectional flow area is a more appropriate length scale since the majority of available data, for a variety of non-circular duct shapes (e.g., rectangular, triangular, annular, elliptical, ect.), can be generalized by a single model when using the appropriate definition of the aspect ratio for the respective geometries.

Due to the relatively short length of the channel in this study, the flow may not become fully developed within a reasonable distance from the inlet. As the velocity profile develops, the flow is changing from a constant velocity at the inlet, into the characteristic parabolic velocity profile due to the non-slip boundary conditions at the walls [25]. Due to the near infinite velocity gradient at the inlet, a sharp increase in the surface shear stress occurs, and hence the friction factor increases dramatically. The velocity profile eventually reaches a steady state or fully developed condition, where, for the case of internal flow, the boundary layers of the walls merge at the centerline of the channel. This situation is depicted in Figure 4-1. How fast the flow develops is dependent on the Reynolds number, and the channel geometry.
Figure 4-1. Schematic of hydrodynamically developing flow (re-created from [25])

The suggested entrance length for flow to become hydrodynamically fully developed is shown by Equation 4.17.

\[ z_{ef.h} = 0.05 \mu Re_L \]  

(4.17)

Instead of fluid transitioning discretely from developing to fully developed flow (as Equation 4.17 demonstrates), one should grasp this process as a more gradual transition as the boundary layer grows and the velocity profile becomes independent of the channel length. A dimensionless length for hydrodynamically developing flow that represents this transition is defined by Equation 4.18.

\[ z^+ = \frac{z}{\mu Re_L} \]  

(4.18)

The most detailed description that was found in literature for hydrodynamically developing flow is from the work of Muzychka and Yavanovich (2002) [58]. Their proposed model for the Fanning friction factor-Reynolds product is presented in Equation 4.19.

\[ f_{\mu} Re_L(z^+) = \left[ \frac{12}{\sqrt{\epsilon} (1 + \epsilon)} \left( \frac{1 - 192 \epsilon}{\pi^2} \tanh \left( \frac{\pi}{2 \epsilon} \right) \right)^2 + \left( \frac{3.44}{\sqrt{z^+}} \right)^2 \right]^{1/2} \]  

(4.19)
The dimensionless position for hydrodynamically developing flow, \( z^+ \), in Equation 4.19 uses the characteristic length based on the square root of the cross-sectional flow area, as shown in Equation 4.20.

\[
z^+ = \frac{z}{\sqrt{A \cdot Re z'}}
\]  

(4.20)

This model may be used to find the friction factor as a function of the channel length, which is needed to find the major head loss, which can subsequently be used to find the total pressure drop along the length of the channel. An example of the characteristics of this model is shown in Figure 4-2 using the cross-sectional flow area of this study and the Reynolds number of 155.9, as calculated previously. The upper horizontal axis is the dimensionless channel length, defined by Equation 4.21, using the channel length of 38 mm (used in this study). For this case, it takes 18.3% of the channel length to reach the recommended hydrodynamic entrance length (Equation 4.17) of \( z^+ = 0.05 \). The value doesn’t reach its fully developed value until several channel lengths. The average Darcy friction factor-Reynolds number product for one channel length for this example is 99.519, compared to the fully developed value of 81.072. Therefore, the flow in this study cannot be assumed to be hydrodynamically fully developed.

\[
\frac{z}{L_{GC}} = \frac{z^+ \sqrt{A \cdot Re z'}}{L_{GC}}
\]  

(4.21)
4.2 Heat Transfer Correlations

The Nusselt number (Equation 4.22) represents the dimensionless temperature gradient at the surface and is defined as the ratio of the convective to pure conductive heat transfer [25]. Similar to the hydrodynamic problem, for internal thermally fully developed laminar flow, the Nusselt number is independent of the channel geometry and fluid properties, but now becomes dependant on the wall boundary condition of the channel. The two most common wall boundary conditions are a uniform wall temperature (denoted by UWT), and a uniform wall heat flux (denoted by UWF). For thermally fully developed laminar flow in a circular channel, the forced convection Nusselt number is $Nu_D = 3.66$ for the UWT boundary condition and is $Nu_D = 4.36$ for
the UWF boundary condition and the characteristic length scale used in Equation 4.22 is the diameter of the circular pipe [3, 25, 55, 56].

\[ Nu_C = \frac{hD_C}{k} \]  \hspace{1cm} (4.22)

For a rectangular channel, the Nusselt number for thermally fully developed laminar flow becomes dependent on the aspect ratio and boundary condition. Several correlations have been given in literature for laminar forced convection heat transfer in non-circular ducts [3, 25, 55-57, 59]. Examples are given below and their values listed for an aspect ratio of 1 and 0.3149 in Table 4-2 for the UWT boundary condition and in Table 4-3 for the UWF boundary condition.

Shah and London (1978, p. 202, p. 205) [56] give the correlations shown in Equations 4.23 and 4.24 for UWT and UWF boundary conditions, respectively.

\[ Nu_f = 7.541 \left( 1 - 2.610 \varepsilon + 4.970 \varepsilon^2 - 5.119 \varepsilon^3 + 2.702 \varepsilon^4 - 0.548 \varepsilon^5 \right) \]  \hspace{1cm} (4.23)

\[ Nu_H = 8.235 \left( 1 - 2.0421 \varepsilon + 3.0853 \varepsilon^2 - 2.4765 \varepsilon^3 + 1.0578 \varepsilon^4 - 0.1861 \varepsilon^5 \right) \]  \hspace{1cm} (4.24)

Bergman, Lavine, Incropera, and Dewitt (2011, p. 553) [25] and Barbir (2005, p. 188) [3] list the values found in Kays and Crawford (1993, p. 125) [55] for the Nusselt numbers for both UWT and UWF boundary conditions as a function of aspect ratio; the values are found through interpolation for the aspect ratio of 0.3149. All of the above correlations are based on using the hydraulic diameter as the characteristic length scale in Equation 4.22, as re-depicted in Equation 4.25.

\[ Nu_D = \frac{hd_n}{k} \]  \hspace{1cm} (4.25)
Table 4-2. Nusselt number for fully developed laminar flow in rectangular channels with varying aspect ratios for a uniform surface temperature wall boundary condition (UWT)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Eq. 4.23</td>
<td>Tabulated</td>
<td>Tabulated</td>
<td>Tabulated</td>
<td>Eq. 4.27*</td>
</tr>
<tr>
<td>$\varepsilon = 1$</td>
<td>2.979</td>
<td>2.980</td>
<td>2.980</td>
<td>2.980</td>
<td>3.229</td>
</tr>
<tr>
<td>$\varepsilon = 0.3149$</td>
<td>4.042</td>
<td>4.044</td>
<td>4.044</td>
<td>-</td>
<td>5.199</td>
</tr>
</tbody>
</table>

*Characteristic length scale based on the square root of cross-sectional flow area

Table 4-3. Nusselt number for fully developed laminar flow in rectangular channels with varying aspect ratios for a uniform heat flux wall boundary condition (UWF)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Eq. 4.24</td>
<td>Tabulated</td>
<td>Tabulated</td>
<td>Tabulated</td>
<td>Eq. 4.27*</td>
</tr>
<tr>
<td>$\varepsilon = 1$</td>
<td>3.610</td>
<td>3.610</td>
<td>3.610</td>
<td>3.610</td>
<td>3.847</td>
</tr>
<tr>
<td>$\varepsilon = 0.3149$</td>
<td>4.903</td>
<td>4.885</td>
<td>4.885</td>
<td>-</td>
<td>6.193</td>
</tr>
</tbody>
</table>

*Characteristic length scale based on the square root of cross-sectional flow area

Shah and London (1978, p. 204) [56] also describe how the number of walls transferring heat affect the Nusselt number. For both UWT and UWF, it is shown that there is a decrease in the Nusselt number when three wall are adiabatic and one wall is transferring heat for all aspect ratios, as depicted in Figure 4-3. Using interpolation of the tabulated values for a UWT, a reduction of 17.95% is found for and aspect ratio of 1 (as used in LaManna (2010) [44]) and a reduction of 11.15% for the aspect ratio in this study of 0.3149.

![Diagram of a rectangular channel with one wall transferring heat and three walls adiabatic](image)

Figure 4-3. Rectangular channel with one wall transferring heat and three walls adiabatic
In continued work by Muzychka and Yavanovich (2004) [59], a model for the Nusselt number is proposed for fully developed laminar flow in non-circular ducts, and successively a correlation for flow with simultaneous developing hydrodynamic and thermal boundary layers. Once again, their model is posed on using the square root of the cross-sectional flow area as the characteristic length scale. Therefore, the Nusselt number based on this characteristic length is shown in Equation 4.26, and the correlation for thermally fully developed flow is presented in Equation 4.27.

\[
Nu_{\sqrt{A}} = \frac{h\sqrt{A}}{k}
\]  

\[
Nu_{\sqrt{A}} = C_1 \left( \frac{f_j Re_{\sqrt{A}}}{8\sqrt{\pi} \varepsilon^2} \right)
\]

Numerical constants for \(C_1\) for the different boundary conditions and the shape parameter, \(\varepsilon\), for a rectangular channel are listed in Table 4-4, and \(f_j Re_{\sqrt{A}}\) is found using Equation 4.16.

Similar to the hydrodynamic velocity boundary layer, a temperature boundary layer must first develop before being considered thermally fully developed flow. As the boundary layer develops the temperature profile is going from uniform at the inlet to a fully developed profile due to the uniform wall condition. This situation is depicted in Figure 4-4 for a uniform wall temperature greater than the fluid inlet temperature. How fast the flow develops is dependent on the Reynolds number, fluid properties and the channel geometry.
Table 4-4. Coefficients for the general model

<table>
<thead>
<tr>
<th>Boundary Condition</th>
</tr>
</thead>
</table>
| UWT               | $C_3 = 0.409$, $C_1 = 3.24$  
|                   | $f (Pr) = \frac{0.564}{1 + \left(1.664 Pr^{0.6}\right)^{9/2}}^{2/9}$  
| UWF               | $C_3 = 0.501$, $C_1 = 3.86$  
|                   | $f (Pr) = \frac{0.886}{1 + \left(1.909 Pr^{0.6}\right)^{9/2}}^{2/9}$  

<table>
<thead>
<tr>
<th>Nusselt Number Type</th>
</tr>
</thead>
</table>
| Local               | $C_2 = 1$, $C_4 = 1$  
| Average             | $C_2 = 3/2$, $C_4 = 2$  

<table>
<thead>
<tr>
<th>Shape Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma = 1/10$</td>
</tr>
</tbody>
</table>

[Figure 4-4. Schematic of thermally developing flow with a uniform wall temperature greater than the fluid temperature (re-created from [25])]
The suggested entrance length for flow to become thermally fully developed is shown by Equation 4.28.

\[ z_{fd,t} = 0.05 \mathcal{L} \text{Re}_t \text{Pr} \]  

(Equation 4.28)

Equation 4.29 recasts the entrance length into a dimensionless position for thermally developing flow, \( z' \). A common parameter for thermally developing flow is the Graetz number, which can be found as the inverse of \( z' \) (Equation 4.30).

\[ z' = \frac{z}{\mathcal{L} \text{Re}_t \text{Pr}} \]  

(Equation 4.29)

\[ Gz = \frac{1}{z'} = \frac{\mathcal{L} \text{Re}_t \text{Pr}}{z} \]  

(Equation 4.30)

The Prandtl number, \( \text{Pr} \), is an important parameter for convective heat transfer as it reflects the ratio of the momentum and thermal diffusivities. It can be understood as a fluids relative ability to transport momentum and energy in the velocity and thermal boundary layers, respectively [25]. The thermal and hydrodynamic entrance lengths are directly related through the Prandtl number (Equation 4.31). For gases, which commonly have a Prandtl number less than 1, the thermal boundary layer develops more quickly than the hydrodynamic boundary layer. In this case, the temperature and velocity boundary layers develop simultaneously to create a combined thermal and hydrodynamic entry length problem.

\[ z_{fd,t} = z_{fd,h} \text{Pr} \]  

(Equation 4.31)

The model that Muzychka and Yavanovich (2004) [59] propose for the Nusselt number for laminar forced convection in the combined entry region of non-circular ducts, is presented in Equation 4.32. The Nusselt number is dependent on the Prandtl number and the dimensionless position for thermally developing flow (Equation 4.33).
\[ Nu_{\frac{A}{\alpha}}(z^*) = \left( \frac{C_4 f(Pr)}{\sqrt{z^*}} \right)^m + \left( C_2 C_3 \left( \frac{f_j Re_{\alpha}}{z^*} \right) \right) + \left( C_1 \left( \frac{f_j Re_{\alpha}}{8 \sqrt{\pi \epsilon \gamma}} \right) \right) \]  
\[ z^* = \frac{z}{\sqrt{A \gamma Re_{\alpha} Pr}} \]  

(4.32)  

(4.33)

Numerical constants \( C_1 - C_4 \) and \( f(Pr) \) are defined in Table 4-4. The blending parameter, \( m \), is dependent upon the Prandtl number based on the approximation given by Equation 4.34. The \( f(Pr) \) term in Equation 4.32 for UWT is shown in Equation 4.35.

\[ m = 2.27 + 1.65 Pr^{1/3} \]  
\[ f(Pr) = \frac{0.564}{\left[ 1 + \left( 1.664 Pr^{1/6} \right)^{9/2} \right]^{2/9}} \]  

(4.34)  

(4.35)

This model may be used to find the local Nusselt number as a function of the channel length, which is needed to find the convection coefficient. An example of the characteristics of this model are shown in Figure 4-5 prepared for the cross-sectional flow area of this study, the Reynolds number of 155.9, and the Prandtl number of 0.7713 corresponding to humid air at 70 °C and 100% RH (from Table A-3). The upper horizontal axis is the dimensionless channel length using the channel length in this study of 38 mm. It takes 14.1% of the channel length to reach the recommended thermal entrance length (Equation 4.28) of \( z^* = 0.05 \). Once again, the value doesn’t reach its fully developed value until several channel lengths. The average Nusselt number for one channel length for this example is 6.410, compared to the fully developed value of 5.199. Therefore the flow in this study cannot be assumed to be thermally fully developed.
4.3 Heat and Mass Transfer Analogy

A direct analogy from heat to mass transfer can be implemented by replacing temperature with concentration. Analogous to the Nusselt number, the Sherwood number (Equation 4.36) represents the dimensionless concentration gradient at the surface and is defined as the ratio of the convective to pure conductive (diffusive) mass transfer [25]. Analogous to the Prandtl number, the Schmidt number, $Sc$, reflects the ratio of the momentum and mass diffusivities. Applying the heat and mass transfer analogy, $Nu$ is replaced by $Sh$ and $Pr$ is replaced by $Sc$ interchangeably [25, 60]. The heat and mass transfer coefficients can also be coupled by assuming that $Nu$ is proportional to $Pr^n$ and $Sh$ is proportional to $Sc^n$, resulting in the Lewis relationship shown in Equation 4.37, where $n = 1/3$ is commonly used.
The heat transfer model shown in Equation 4.32 for finding the Nusselt number [58, 59] may be recast for mass transfer to find the Sherwood number based on the square root of the cross-sectional flow area as the characteristic length (Equation 4.38), as presented in Equation 4.39.

\[
Sh_{\sqrt{A}} = \frac{h_m\sqrt{A}}{D_{AB}} \tag{4.38}
\]

\[
Sh_{\sqrt{A}}(z^-) = \left[ \left( \frac{C_4 f(Sc)}{\sqrt{z^-}} \right)^m + \left\{ C_2 C_3 \left( \frac{fRe_{\sqrt{A}}}{z^-} \right)^{1/3} \right\}^5 + \left\{ C_1 \left( \frac{fRe_{\sqrt{A}}}{8\sqrt{\pi} \varepsilon^2} \right) \right\}^5 \right]^{1/m} \tag{4.39}
\]

Since it was shown above that temperature profile would not be fully developed, the concentration profile will follow a similar trend. Equation 4.40 shows the dimensionless positon for flow with a developing concentration boundary layer, \( z^- \), where the characteristic length is based on the square root of the cross-sectional flow area.

\[
z^- = \frac{z}{\sqrt{A_{\text{Re}} \sqrt{A} Sc}} \tag{4.40}
\]

The blending parameter, \( m \), is now dependent upon the Schmidt number (Equation 4.41), and the \( f(Sc) \) term in Equation 4.39 for UWT is shown in Equation 4.42.

\[
m = 2.27 + 1.65 Sc^{1/3} \tag{4.41}
\]

\[
f(Sc) = \frac{0.564}{\left[ 1 + \left( 1.664 Sc^{1/6} \right)^{9/2} \right]^{2/9}} \tag{4.42}
\]
CHAPTER 5: ANALYTICAL MODEL

This chapter presents the analytical model used for extracting the effective water vapor diffusion coefficient of the GDL from the experimental data obtained. Section 5.1 provides a detail description of the physical processes of the model and includes a schematic encompassing the problem statement. The general rationale and procedure used to solve the model will then be explained. Assumptions of the model are stated in Section 5.2 and are later validated in Section 5.5. The primary governing equations defining the underlying physics are derived for the water vapor diffusion model in Section 5.3. Section 5.4 presents the final theoretical solution for the model for a set of standard inputs. Section 5.6 explains how the diffusion coefficient is extracted from the experimental results using the model.

5.1 Schematic and Procedure

A schematic of the analytical model is shown in Figure 5-1. Liquid water is placed on top of the GDL with a dry (or partially humidified) air stream flowing through an internal channel below. The liquid water is evaporated and then diffuses through the GDL by means of water vapor diffusion. The rate of water removal may be found by employing a model that accounts for the mechanisms of transport (i.e., water vapor diffusion via concentration difference). This can be achieved by deriving the fundamental equations for the principals driving mass transfer and evaluating these relationships along the length of the flow channel.

As the dry (or partially humidified) air flows down the channel, it continually becomes more humid as water is transported through the GDL into the air stream. This concentration change will lead to a change in the thermophysical properties of the gas mixture. A detailed evaluation on the effect of temperature (between 0-100°C) and humidity levels (between dry and saturated) on thermophysical and transport properties is given by Tsilingiris (2008) [61] and is reviewed in
Appendix A. These correlations will be used to solve for the properties of humid air as they change along the channel length.

![Schematic of analytical model](image.png)

**Figure 5-1.** Schematic of analytical model

The water vapor must first transport through the GDL (via mass diffusion) and then transport into the gas channel (via mass convection). In order to separate the water vapor diffusion coefficient of the GDL from the total water vapor transport resistance (diffusion + convection), a convective mass transfer coefficient must be found. Using heat and mass transfer analogy, this coefficient is solved for using the principles explained in literature. Muzychka and Yocanovich (2002, 2004) [58, 59] provide correlations for simultaneously developing laminar flow. The correlations for forced convection friction factors and heat transfer coefficients for rectangular ducts are used to obtain the local convective mass transfer coefficient along the channel length.

Governing equations for a differential element of the geometry are derived based on the principals and correlations provided, with guidance from Bergman, Lavine, Incropera, and Dewitt (2011) [25]. The geometry is then discretized along the channel length, with each segment having a known inlet condition and solving for the outlet condition. The rate of water removal through the GDL as a function of the channel length can be evaluated using this one dimensional model.
5.2 Assumptions

The assumptions that are made for the model are listed below. The validity of the assumptions are discussed in Section 5.5.

a) Isothermal condition (i.e., effect of evaporative cooling is minimal)
b) Ideal gas behaviour
c) Steady state condition
d) Laminar flow
e) Incompressible flow
f) Single phase water vapor transport (i.e., no condensation)
g) No advection through the GDL
h) Through-plane diffusion only
i) Single channel

5.3 Water Vapor Diffusion Model

The channel is discretized into finite elements and the derivation for the model is performed on a single differential element, and then integrated along the channel length from the inlet to the outlet to find the rate of water transport through the GDL as a function of the channel length. The flux of water vapor (per unit area) that diffuses through the GDL from the water side to the interface of the GDL and air channel can be found using Fick’s first law of diffusion, as shown in Equation 5.1. The driving potential is the gradient of water vapor density (concentration) across the thickness of the GDL (from the water side to the GDL/gas channel interface).

\[
J_v = \frac{D_{eff}}{H_{GDL}} (\rho_{v,s} - \rho_{v,H_{GDL}})
\]  

(5.1)

Compared to the binary water vapor/air diffusion coefficient, the effective diffusion coefficient is used to account for the decrease in diffusion that occurs due to the additional resistance of the porous GDL. The normalized diffusion coefficient represents the fraction of the effective
diffusion coefficient to the binary diffusion coefficient (Equation 5.2), thus indicating the fraction
the porous layer is contributing to the decrease in diffusion. This decrease is due to the intrinsic
properties of the GDL (i.e., porosity, pore size distribution). The normalized diffusion coefficient
should remain constant in an individual sample when a different binary gas mixture is used or the
temperature changes (since the binary diffusion is dependent on temperature).

\[ D_{\text{norm}} = \frac{D_{\text{eff}}}{D_{v,a}} \]  

(5.2)

The flux of water vapor through the GDL, given in Equation 5.1, must be equal to the flux of water vapor entering the air channel. This occurs by means of forced convective mass transfer. Using Newton’s law of cooling (converted from heat to mass transfer), this rate is defined in Equation 5.3, using the driving potential as the gradient of water vapor density from the interface of the GDL/gas channel to the average free stream density of the humid air flow in the channel. The mass transfer coefficient represents the conductance (or resistance) that is provided from the motion of fluid (air) and is dependent on the conditions of the boundary layer (which is influenced by the geometry) and the thermophysical and transport properties of the fluid.

\[ j_v = h_m \left( \rho_v \bigg|_{y=H_{GC}} - \bar{\rho}_{v,\text{flow}} \right) \]  

(5.3)

Combining Equations 5.1 and 5.3, the rate of water vapor removal through the GDL is presented in Equation 5.4.

\[ j_v = \left( \rho_{v,s} - \bar{\rho}_{v,\text{flow}} \right) \left( \frac{H_{\text{GDL}}}{D_{\text{eff}}} + \frac{1}{h_m} \right) \]  

(5.4)

Considering Equation A.2, \( \rho_v = \frac{P_v}{R_v T} \), and Equation A.7, \( \phi = \frac{P_v}{P_s} \), Equation 5.4 is redefined in Equation 5.5.
\[
 j_v = \frac{P_v}{RT} \left(1 - \bar{\phi}\right) \left( \frac{H_{GDL}}{D_{eff} h_m(z)} + \frac{1}{h_m(z)} \right)
\]

Equation 5.5 follows the typical resistance network concept, in which the rate of transfer is represented by the ratio of a driving potential to the total resistance. For certain problems (such as in heat exchangers), the log mean difference is commonly used for the driving potential, which relies on only the inlet and outlet conditions. This heat exchanger analysis method is also restricted to using average values for heat or mass transfer coefficients and solving for fluid properties at a specific constant temperature (usually the film temperature which is the average temperature of the wall and flow). For these reasons, this method was not used. Instead, for a more accurate analysis, the discretization of differential elements and integration along the channel length are employed using a generalized finite element method. The differential elements had a resolution of 20 cells/mm, or a step size of 0.05 mm. This divides the 38 mm long channel into 760 elements.

Since water is continually diffusing into the channel, the water vapor content of the humid air flow will increase. The mass transfer coefficient is also a function of the channel length and the humid air properties (mainly the Schmidt number). Equation 5.6 is used to solve for the flux of water vapor transport through the GDL as a function of the channel length.

\[
 j_v(z) = \frac{P_v}{RT} \left(1 - \phi_{v,\text{flow}}(z)\right) \left( \frac{H_{GDL}}{D_{eff} h_m(z)} + \frac{1}{h_m(z)} \right)
\]

The local convective mass transfer coefficient, \( h_m(z) \), is found using Equation 4.38, where the local Sherwood number is found using Equation 4.39. As there is a liquid water chamber on the one side of the GDL, the boundary condition for finding the Sherwood number in the model is a
constant wall concentration (analogous to uniform wall temperature; UWT). The local Sherwood number is of interest, therefore appropriate constants $C_1 - C_4$ are chosen. This Sherwood number must be reduced by 11.15% since only one wall is transferring mass while the other three are adiabatic. The Schmidt number is found according to the local water content of the air (using the method described in Section A.2 of Appendix A).

The inlet humidity ratio is found using the known inlet RH. Once the flux of water vapor is found for an element, the rate of water vapor transport can be found using Equation 5.7. The humidity ratio for the next element can be determined using Equation 5.8, and the RH using Equation 5.9.

$$\dot{m}_{v,i} = j_{v,i}(z) \cdot W_{GC} \cdot \Delta z \quad (5.7)$$

$$\omega_{t+1} = \omega_t + \frac{\dot{m}_{v,i}}{\dot{m}_a} \quad (5.8)$$

$$\phi_{t+1} = \frac{P}{P_s \left(1 + \frac{0.6219}{\omega_{t+1}}\right)} \quad (5.9)$$

Since the pressure drop is initially unknown, a preliminary iteration solves the model using a constant atmospheric pressure while simultaneously solving for the pressure drop of each section (using the method outlined in Section 4.1 of Chapter 4). The model is iterated using the known pressure drop along the length of the channel until convergence is found.

### 5.4 Model Solution

Figure 5-2 show a flow diagram of the method used to solve the model. An algorithm was written in MATLAB which solves for the pressure drop, RH concentration profile, and corresponding humid air properties along the length of the channel with known input conditions.
Figure 5-2. Flow diagram for analytical model
The model was solved using the parameters shown in Table 5-1. Figure 5-3 shows the resulting RH profile along the length of the channel. Figure 5-4 shows the resulting pressure drop along the length of the channel, which matches well with the pressure drops found in Sections 2.3.1 and 3.4.

### Table 5-1. Inputs to analytical model

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet air RH</td>
<td>35%</td>
</tr>
<tr>
<td>Inlet dry air flow rate</td>
<td>$1.8938 \times 10^{-6}$ kg/s</td>
</tr>
<tr>
<td>Temperature</td>
<td>70°C</td>
</tr>
<tr>
<td>Saturation pressure</td>
<td>31180 Pa</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>101325 Pa</td>
</tr>
<tr>
<td>$D_{norm}$</td>
<td>0.15</td>
</tr>
<tr>
<td>$D_{v,a}$</td>
<td>0.3213 cm$^2$/s</td>
</tr>
<tr>
<td>$D_{eff}$</td>
<td>0.0482 cm$^2$/s</td>
</tr>
<tr>
<td>$H_{GDL}$ (uncompressed)</td>
<td>190 μm</td>
</tr>
<tr>
<td>$H_{GC}, W_{GC}, L_{GC}$</td>
<td>0.5, 1.588, 38 mm</td>
</tr>
</tbody>
</table>

*Figure 5-3. Relative humidity along the dimensionless channel length*
5.5 Validity of Assumptions

The validity of the assumptions made in Section 5.2 are discussed below:

(a) Isothermal condition (i.e., effect of evaporative cooling is minimal)

Since water is changing from a liquid state to a vapor state, there will be a certain amount of heat required for the phase change. This can cause evaporative cooling of the air if no other heat is added. The coolant plates supply this heat such that the air temperature doesn’t drop from the inlet to the outlet. For the case studied here, the total mass of rate of water removal for the entire active area is $1.2 \times 10^{-6}$ kg/s. Using a latent heat of vaporization for water at 70°C of 2333.8 kJ/kg, the amount of heat that should be added is 2.8 W. Since the coolant water flows at 0.0894 kg/s, it only needs to change a fraction of a degree (0.0075°C) to supply this heat, using the specific heat for water at 70°C of 4.190 kJ/kg/K. This proves that the effect of evaporative cooling is minimal.
(b) Ideal gas behaviour

The total pressure is kept well below 3 atmospheres and, hence, the air will obey the ideal gas law with sufficient accuracy for the current applications [62].

(c) Steady state condition

Steady state was assumed for the theoretical model since no transient effects were of interest. The experimental results were obtained during steady state.

(d) Laminar flow

The maximum Reynolds number in the channel for the solved case was 131, proving that it falls well below 2300, and the flow is therefore laminar.

(e) Incompressible flow

The maximum humid air mixture velocity in the channel for the case studied here was 2.86 m/s, proving that it falls well below a Mach number of $Ma = 0.3$ (102 m/s), and the flow is therefore incompressible.

(f) Single phase water vapor transport (i.e., no condensation)

Only low RH air input conditions were used for the model ($\leq 35\%$ RH). The higher dewpoint temperature of the more humid conditions may cause condensation to occur.

(g) No advection through the GDL

Since the pressure from the air side to the water side is balance (using the pressurized water columns), no advection (or permeation of liquid water) should occur through the GDL. The maximum height of the water column is ~10 cm, which creates 1000 Pa of hydrostatic pressure at the MPL surface. Since the MPL is hydrophobic, this pressure does not overcome the capillary pressure needed for liquid water permeation through a GDL with an MPL [40, 26].
(h) Through-plane diffusion only

The resistance for water vapor to diffuse down the open channel length is much greater than the resistance for water vapor to diffuse through the GDL. For example, taking the ratio of the channel length (38 mm) to the diffusivity of water vapor at 70°C of 0.3213 cm²/s leads to a resistance of 11.84 s/cm. However, taking the ratio of the GDL thickness (190 μm) to the effective diffusivity of water vapor in the GDL at 70°C of 0.0482 cm²/s leads to a resistance of 0.42 s/cm. Therefore, diffusion is much more likely to occur in the through-plane direction of the GDL, rather than diffusing in the in-plane direction of the GDL or down the channel.

(i) Single channel

As there is no concentration gradient driving water removal under the lands, diffusion is neglected in these regions. This is valid since, for the setup in the study, the liquid water chamber does not allow water to sit directly above the lands, only above the channel area.

5.6 Extracting the Water Vapor Diffusion Coefficient of the GDL from Experimental Data

The only unknown in the model is the effective water vapor diffusion coefficient of the GDL. The experimental inlet conditions as well as the uncompressed thickness of the GDL are input to the model and it is solved for a range of diffusion coefficients. The final diffusion coefficient is found using a least squared method to minimize the residual error between the experimental RH points and the theoretical RH found using the model. This effective water vapor diffusion coefficient represents the best fit between the experimental and theoretical results.
CHAPTER 6: RESULTS AND DISCUSSION

The results for the in-situ experiment are presented in Section 6.1. Included are the polarization curves and constant current power output for the set of input conditions. The results for the quasi in-situ experiment are presented in Section 6.2. Included are the rate of water removal of the five sections and the water vapor concentration (RH) profile along the channel length for the same set of input conditions. The final effective water vapor diffusion coefficient for the GDL extracted from the model using the experimental data will be also reported. In Section 6.3, the results from the condenser and estimated outlet water contents (RH) for the two types of experiments will be presented and discussed in relation to one another. Throughout this chapter, consideration will be given to the implications of these findings.

6.1 In-situ

Figure 6-1 shows the voltage versus current density polarization curves for the eight test conditions. Recall that the points are presented as box plots of the recorded current data for each constant voltage step. The black marker is the median, the green errors bars denote the 25 and 75 percentiles, and the red error bars mark the minimum and maximum. Figure 6-2 displays the voltage versus current density and power density versus current density polarization curves. Figure 6-2(a) is for the low stoichiometric flow rate (i.e., $\lambda_{o2} = 3$ at 1 A/cm$^2$), and Figure 6-2(b) is for the high stoichiometric flow rate (i.e., $\lambda_{o2} = 6$ at 1 A/cm$^2$). Figure 6-3 provides a subplot of the chronopotentiometric performance at a constant current of 1 A/cm$^2$ for all of the input conditions. Table 6-1 quantifies the means and standard deviations of the power density output from the constant current test runs displayed in Figure 6-3. To facilitate the visual presentation of these results, Figure 6-4 displays the boxplots obtained for these runs. These figures will be referred to in the ensuing paragraphs which discuss the results.
Figure 6-1. Subplot of voltage versus current density polarization curves for all input conditions.
Figure 6-2. Voltage versus current density (left axis) and power density versus current density (right axis) polarization curves for all RH input conditions at (a) the low stoichiometric flow rate (i.e., $\lambda_{O_2} = 3$ at 1 A/cm$^2$), and (b) the high stoichiometric flow rate (i.e., $\lambda_{O_2} = 6$ at 1 A/cm$^2$)
Figure 6-3. Subplot of constant current of 1 A/cm² versus time for all input conditions
Table 6-1. Power density for a constant current density of 1 A/cm²

<table>
<thead>
<tr>
<th>Flow rate</th>
<th>Inlet air relative humidity</th>
<th>35%</th>
<th>65%</th>
<th>95%</th>
<th>125%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low ( \lambda_2 = 3 \text{ at } 1 \text{ A/cm}^2 )</td>
<td>0.432 (0.020)</td>
<td>0.120 (0.122)</td>
<td>0.215 (0.154)</td>
<td>0.199 (0.193)</td>
<td></td>
</tr>
<tr>
<td>High ( \lambda_2 = 6 \text{ at } 1 \text{ A/cm}^2 )</td>
<td>0.454 (0.006)</td>
<td>0.470 (0.009)</td>
<td>0.438 (0.020)</td>
<td>0.445 (0.013)</td>
<td></td>
</tr>
</tbody>
</table>

Note. Means are reported with standard deviations in brackets. All results are statistically different from one another at a significance level of \( p < .001 \).

Figure 6-4. Box plot of power density at constant current density of 1 A/cm²

6.1.1 Effect of flow rate

A factorial ANOVA indicated a significant main effect of flow rate on power density, \( F(1, 71216) = 80538.57, p < .001, \eta^2 = .53 \). As can be seen across both characterization techniques (i.e., the polarization curve and constant current), all of the high stoichiometric flow rates produce better performance than the low stoichiometric flow rates for the same humidity level. That is, as the
flow rate increases, so does the power density output. As indicated by Figure 6-1, the higher flow rates not only outperform the lower flow rates, they also demonstrate significantly less fluctuation, especially at high current densities. This was expected, as a higher flow rate causes a lower drop in oxygen concentration along the channel which increases oxygen diffusivity. However, with an oxygen stoichiometry greater than approximately three, the outlet oxygen concentration remains relatively constant \[3\]. Since the oxygen stoichiometry was kept above three in this study, oxygen starvation may not be the primary performance factor. Instead, this improvement in performance and stability may be attributable to the increased water removal capabilities inherent with faster channel velocities.

6.1.2 Effect of relative humidity

The factorial ANOVA also indicated a significant main effect of RH on power density, \(F(3, 71216) = 7852.35, p < .001, \eta^2 = .25\). The Bonferroni post hoc analyses \[51, 52\] revealed that all RH conditions significantly differ from one another (all \(p \text{s} < .001\)). Overall, increasing the humidity of the air decreases performance, with the 35% RH condition attaining the greatest performance on average. Further, at the low flow rate, more fluctuation occurs as the relative humidity increases (as can be seen in Figure 6-1). This improvement in stability at lower RH levels may be explained by higher rates of water removal caused by higher water vapor concentration gradients. At the high flow rate, relative humidity does not appear to affect stability. As may be noticed by examining the figures and table above, the interpretation of the effect of RH is complicated by the interaction between flow rate and RH.

6.1.3 Interaction effect between flow rate and relative humidity

The factorial ANOVA indicated a significant interaction effect between flow rate and RH on power density, \(F(3, 71216) = 8471.93, p < .001, \eta^2 = .26\). This indicates that the effect of RH
on the power density output was dependent on which flow rate was used. Although Bonferroni post hoc analyses [51, 52] indicated that the power densities from all of the conditions were statistically different from one another (all ps < .001), the mean differences between conditions varied. Specifically, the mean differences in power density were very small across all RH conditions for the high flow rate, ranging from 0.007 to 0.032 W/cm². However, for the low flow rate, the mean differences in power density between the 35% RH condition and each of the higher RH conditions were larger (range: 0.217-0.312 W/cm²) than the mean differences between the three highest RH conditions (range: 0.016-0.095 W/cm²). These differences can be interpreted qualitatively by examining Figure 6-4.

Notably, the 35-3 condition achieved similar performance to that achieved by all of the high flow rate conditions. The distinct performance of this combination may be due, in part, to the higher water vapor concentration gradient between the CL and flow channel, which produces water removal capabilities sufficient to prevent flooding even at high current densities. In accordance with this explanation, the high fluctuations and poor performance seen in Figure 6-1 for the 95-3 and 125-3 conditions can be attributed to insufficient water removal capabilities, which cause flooding in the CL, GDL, and/or flow channels. Based on these results, we can conclude that although the high flow rate achieves greater performance and stability overall, the air flow rate has less of an influence on performance when the humidity level of the air is decreased to 35%.

6.1.4 Summary of in-situ performance

To summarize the results from the chronopotentiometric in-situ testing, there is a significant positive relationship between flow rate and performance, as well as a significant negative relationship between RH and performance. There is also a significant interaction between flow rate and RH, such that the positive effect of flow rate on performance is greatest at the three
highest RH levels. There is only a slight increase in the power density output between 35-3 and 35-6 conditions. Importantly, the effect size of flow rate exceeds the effect size of either RH or the interaction term, attesting to its importance for fuel cell performance. The highest performance was demonstrated by the 65-6 condition (inlet air RH of 65% and high flow rate), which obtains a power density of 0.470 W/cm$^2$ at 1 A/cm$^2$. In contrast, the lowest performance was observed for the 65-3 condition, followed by the 125-3 and 95-3 conditions, which all obtain power densities below 0.215 W/cm$^2$.

The trends found using chronopotentiometry at 1 A/cm$^2$ are reflected in the high current density region of the polarization curves. However, it is also evident from the polarization curves (Figure 6-2) that drier air inputs achieve worse performance in the low current density region, indicating increased ohmic resistance due to drying of the PEM. It is worth mentioning that the peak power occurred at the 0.45 V step across all conditions (see Figure 6-2). For the majority of the test conditions, the current density at the peak power was ~1 A/cm$^2$. Hence, the results obtained during the constant current performance testing reflect the cell’s performance at its peak power.

Although output power is important, other factors should be considered in choosing ideal operating conditions. For example, higher flow rates result in increased parasitic pumping losses, which decreases the net power produced by a system. In addition, higher humidity levels require balance-of-plant components, which can add complexities to the system. Stability should also be considered. Hence, although the 65-6 condition achieved the greatest performance in lab, the 35-3 and 35-6 conditions may be preferred in practice considering their similar performance and stability as well as their reduced expenditures, especially for fuel cell stack designs.
6.2 Quasi In-situ

The nine quasi in-situ tests are listed in Table 6-2, which encompass the same operating conditions as that of the in-situ experiment, as well as tests for repeatability and model validation. Tests 1-3 are repeats for the 35% RH condition. The ID of the water column was changed in the last test to validate that the size of water column had no effect on the final results of the experiment. Tests 4-7 cover the remaining flow rate and RH combinations for a 70°C cell temperature, with a repeat of the 65% RH conditions. Tests 8 and 9 were run with inputs chosen for model validation.

Table 6-2. Conditions for quasi in-situ tests

<table>
<thead>
<tr>
<th>Test number</th>
<th>Cell temperature</th>
<th>Flow rate</th>
<th>Inlet relative humidity</th>
<th>ID of water column</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>70°C</td>
<td>Low, High</td>
<td>35%</td>
<td>3/32”</td>
</tr>
<tr>
<td>2</td>
<td>70°C</td>
<td>Low, High</td>
<td>35%</td>
<td>3/32”</td>
</tr>
<tr>
<td>3</td>
<td>70°C</td>
<td>Low, High</td>
<td>35%</td>
<td>4/32”</td>
</tr>
<tr>
<td>4</td>
<td>70°C</td>
<td>Low, High</td>
<td>65%</td>
<td>3/32”</td>
</tr>
<tr>
<td>5</td>
<td>70°C</td>
<td>Low, High</td>
<td>65%</td>
<td>3/32”</td>
</tr>
<tr>
<td>6</td>
<td>70°C</td>
<td>Low, High</td>
<td>95%</td>
<td>2/32”</td>
</tr>
<tr>
<td>7</td>
<td>70°C</td>
<td>Low, High</td>
<td>125%</td>
<td>2/32”</td>
</tr>
<tr>
<td>8</td>
<td>70°C</td>
<td>Low</td>
<td>10%</td>
<td>4/32”</td>
</tr>
<tr>
<td>9</td>
<td>50°C</td>
<td>High</td>
<td>35%</td>
<td>2/32”</td>
</tr>
</tbody>
</table>

6.2.1 Water removal rates

Figure 6-5 shows a subplot of the water removal rates for the five water columns for each of the main test conditions (i.e., those used in the in-situ experiments). For the 35% and 65% RH plots, the average of the repeated test runs is displayed. As expected, the low flow rate resulted in lower capabilities of water removal across all conditions, except for at the highest humidity level. For the 125% RH conditions, both flow rates obtained similar water removal rates, which is
consistent with findings from past studies [41] and is most likely due to the lack of a concentration gradient. Despite this lack of driving potential, some water removal still occurred at statistically significant levels. Also, in accordance with our expectations, higher capabilities of water removal were evident as RH decreased. This effect can be explained by the increasing concentration gradient present with lower levels of humidity. Finally, there was a consistent water vapor diffusivity trend along the length of the flow channels, such that the sections near the inlet had a higher rate of water removal as compared to the sections near the outlet. This tapering effect is due to the continual increase in RH as water is added to the air stream along the channel length, which results in less water vapor diffusion in the latter segments of the flow field.

In Figure 6-6, the total water removal rate for each of these conditions is compared to one another. The amount of water generated at an equivalent current density of an operational fuel cell is denoted on the right axis \( I_{eq} = \left( \frac{\dot{m}_w - 2F}{M_{H_2O}} \right) \); the in-situ water production rate (Equation 3.6) at a constant current density of 1 A/cm² is marked with a purple line (neglecting osmotic drag and back diffusion). As revealed in this figure, the 35-3 and 35-6 conditions produce a removal rate that greatly surpasses the production rate at 1 A/cm². This indicates that sufficient water is being removed to prevent flooding, which helps explain the advantageous performance obtained by these conditions during in-situ testing. The rate of water removal for the 65-6 condition corresponds with the purple line, which suggests that this condition obtains an optimal water balance and may help explain why this condition achieves the highest in-situ performance results. In contrast, for the 65-3 condition a much lower rate of water was removed, which corresponds to the decreased in-situ performance. The low performance obtained by the 95-3 and 125-3 conditions is consistent with this explanation. However, the good performance achieved by the 95-6 and 125-6 conditions contradict this explanation, which will be discussed further in Section 6.3.
Figure 6-5. Rates of water removal for the five sections
Figure 6-6. Total rates of water removal for the quasi in-situ test conditions

Note. The purple line represents the in-situ water production rate at 1 A/cm\(^2\).

### 6.2.2 Water vapor diffusion coefficient of the GDL

The normalized effective water vapor diffusion coefficient of the GDL was extracted from the model (explained in Chapter 5) for Tests 1-3. The results from the model fit are listed in Table 6-3. Strong repeatability is demonstrated between the runs. The final average coefficient from these tests is 0.1497. Since the diffusion coefficient for water vapor in air is 0.3213 cm\(^2\)/s at 70°C, the final effective water vapor diffusion coefficient of the studied GDL with an MPL is 0.0481 cm\(^2\)/s at 70°C. This value is consistent with values reported in literature [40, 42, 43]. This final diffusion coefficient represents the total resistance of both the MPL and carbon fiber substrate of the GDL. Since the MPL has a small pore size (< 500 nm), the final diffusivity also includes the effects of Knudsen diffusion [63].

This average diffusion coefficient was then used to re-solve the model, using the average input conditions from Tests 1-3. The resulting theoretical RH concentration profile and the average...
of the experimental points are displayed in Figure 6-7(a). There is excellent agreement between the theoretical model and the experimental points. To test the predictive ability of the model, the final normalized diffusivity was fixed in the model and the model was re-solved for the inputs of Tests 8 and 9. Test 8 confirms that a drier RH condition adheres to the model, while Test 9 proves that the normalized diffusion coefficient remains consistent across cell temperatures. Once again, the experimental points are predicted with high accuracy, as shown in Figure 6-7(b). For higher humidity inputs (i.e. ≥ 65% RH) the model validity decreases since liquid water may be present (see validity of assumption (f) in Section 5.5).

It is important to note that the normalized effective diffusion coefficient represents the fraction of diffusivity compared to that of binary diffusion. Therefore, for the lower cell temperature of 50°C used in Test 9, the binary diffusion coefficient of water vapor in air decreases to 0.2936 cm²/s. Therefore, the final effective water vapor diffusion coefficient of the studied GDL with an MPL decreases to 0.0440 cm²/s at 50°C. In research conducted by Tahseen (2013) [49], oxygen diffusivity was found for this particular GDL sample. The researchers found an effective oxygen diffusion coefficient of 0.0275 cm²/s at ~25°C. Using a binary diffusion coefficient of 0.170 cm²/s, a normalized effective diffusion coefficient in the range of 0.160 to 0.170 for this GDL was reported, which is comparable to the value of 0.1497 obtained in the current study.

<table>
<thead>
<tr>
<th>( D_{\text{norm}} )</th>
<th>Test number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow rate</td>
<td>1</td>
</tr>
<tr>
<td>Low ( (\lambda_{\text{O}_2} = 3 \text{ at 1 A/cm}^2) )</td>
<td>0.152 ± 0.019</td>
</tr>
<tr>
<td>High ( (\lambda_{\text{O}_2} = 6 \text{ at 1 A/cm}^2) )</td>
<td>0.153 ± 0.008</td>
</tr>
</tbody>
</table>

*Note.* Averages and ±95% confidence intervals are reported.
Figure 6-7. Experimental and theoretical relative humidity as a function of dimensionless channel length for (a) the average of Tests 1-3, and (b) Tests 8 and 9

Note. The first number in the legend labels denotes the cell temperature (e.g., ’50-35-6’ was the 35% RH inlet air and high flow rate condition run at a 50°C cell temperature)
6.3 Water Removal Comparison Between In-situ and Quasi In-situ Experiments

The outlet humidity of the cathode air for the in-situ experiment was assessed using the rate of water collection from the liquid water trap and condenser during the constant current testing. From this, the outlet humidity of the anode hydrogen was calculated, using the known water production rate, as well as the known inlet and outlet flow rates (as described in Section 3.5.1). The differences between the inlet and outlet RH levels as a function of the inlet air RH are presented in Figure 6-8 for both the cathode and anode. Figure 6-8(a) displays the results for the low air flow rate and Figure 6-8(b) displays the results for the high air flow rate. The difference between the inlet and outlet for the air in the quasi in-situ experiment is overlaid on these graphs. The juxtaposition of the relative humidity difference trends exemplifies the relationship between the cathode and anode water transport. Further, this presentation format facilitates comparison of the water removal capabilities obtained for the quasi in-situ air and in-situ cathode air, which provides a useful link between the in-situ and quasi in-situ results.

Regarding the low flow rate results shown in Figure 6-8(a), the humidity level of the outlet cathode air for the in-situ experiment remains statistically similar to that of the outlet air for the quasi in-situ experiment for all inlet RH conditions ($t(22) = -0.003$, $p = .979$). This similarity suggests that the same amount of water is being removed by the air stream for both types of experiments. As can be seen, the anode RH differences from the inlet to the outlet increase substantially for the higher RH conditions (above 35% RH), while the cathode RH differences for these conditions remain low. Recall the results from the quasi in-situ experiment showing that the rate of water removal falls well below the rate of water production at 1 A/cm$^2$ for RH levels above 35% at the low flow rate (Figure 6-6).
Figure 6-8. Difference in relative humidity from the inlet to outlet for the anode and cathode of the in-situ testing and air for the quasi in-situ testing for (a) low flow rate, and (b) high flow rate.
Considering this insufficient water removal, water should start to accumulate at the cathode and create a flooded state during these conditions for the in-situ experiment. The high liquid water content at the cathode causes back diffusion from the cathode to the anode to ensue, which promotes flooding at the anode. This explanation adheres to the increase in the anode RH of ~35% (from 100% to 135%) for RH conditions above 35% (see Figure 6-8(a)). In essence, the poor in-situ performance across these conditions can be attributed to flooded pathways blocking reactant diffusion to both of the electrodes’ CLs. However, for the 35-3 condition, sufficient water is removed by the drier air stream. Thus, no flooding occurs and good in-situ performance is obtained. Accordingly, the anode RH only increases ~10% for this condition.

Regarding the high flow rate results shown in Figure 6-8(b), the humidity level of the outlet cathode air for the in-situ experiment statistically deviates from that of the outlet air for the quasi in-situ experiment for all inlet RH conditions ($t(22) = 2.36, p < .05$). This deviation indicates that more water is being removed by the cathode air of the in-situ experiment as compared to the air of the quasi in-situ experiment. This increased water removal by the cathode air is reflected in the anode RH differences, which reveal a decrease in RH for the driest condition and only slight increases for the more humid conditions. Figure 6-6 indicates that the rate of water removal due to vapor diffusion meets or exceeds the rate of water production at 1 A/cm² for the 35-6 and 65-6 conditions. Considering this sufficient water removal, no flooding should occur for these conditions, which can account for their good performance. Along these lines, one would expect the 95-6 and 125-6 conditions to perform poorly given their lower rates of water removal found during quasi in-situ testing (see Figure 6-6). However, the fact that these conditions performed on par with the drier conditions is explicable given that the cathode air RH differences are much higher than the quasi in-situ air RH differences (see Figure 6-8(b)). The reason for this difference,
while not fully understood, may be that the reaction is producing both liquid water and water vapor, whereas the quasi in-situ experiment contains solely liquid water. The increased flow rate appears to positively affect the cathode air water removal capabilities during in-situ operation. This increase in water removal rates, or increase in cathode RH differences from the inlet to the outlet, prevents flooding in the cell. Hence, good performance is seen across all RH levels for the high flow rate (see Figure 6-3).

For the quasi in-situ setup, the rate of water collected by the condenser should be equivalent to the amount of water in the input air plus the amount of water removed from the columns. To confirm this, the total amount of water entered into the system was compared to the output rate from the condenser (i.e., water out of the system) and the results were statistically equivalent across all input conditions. It should be noted that the error bars for the in-situ RH data using the condensed output air method are quite large (± 9% max.). Even after rigorous testing and troubleshooting for noise reduction, condensing the output air is prone to several experimental errors, which are commonly not mentioned in other studies that employ a similar method [36-39, 26]. Together, these errors are further amplified by the sensitivity of the system of equations used for analysis. In comparison, the quasi in-situ testing is much more accurate, predicting the outlet RH within ±3% (max.), which is comparable to using RH sensors (±2%) [40, 41-44].

To summarize the relationship between the in-situ and quasi in-situ experiments, we found that when the quasi in-situ water removal rates are above the water production rate at 1 A/cm², good in-situ performance is obtained. The quasi in-situ experiment is limited for the 95-6 and 125-6 conditions as it may not completely capture in-situ water removal processes under these conditions. Despite this limitation, the quasi in-situ method provides a novel approach to finding the effective water vapor diffusion coefficient of the GDL with excellent precision. It also aids in
the interpretation of local flooding characteristics along the length of the flow field by yielding more detailed spatial information about water transport than that which can generally be obtained by in-situ experiments, while also employing more realistic operating conditions than those that can generally be achieved by ex-situ experiments. Jointly, the in-situ and quasi in-situ experiments offer a rich characterization of water management within PEMFCs.
CHAPTER 7: CONCLUSIONS

For this thesis, an experimental setup was designed and manufactured for the purposes of investigating water transport in a PEMFC during operation. Prior to manufacturing, rigorous design work was implemented to ensure the proper operation of the assembled setup. This included simulating the flow of the fluids in the reactant and air flow plates as well as the coolant plates to achieve an even distribution across the flow fields. An analytical model was developed to precisely extract the effective water vapour diffusion coefficient of the GDL from experimental results. Two types of experiments, in-situ and quasi in-situ, were used in parallel to characterize in-situ PEMFC performance and capture the local rates of water removal through the GDL along the length of the flow field across a variety of input air conditions. Two water removal processes were of interest: water vapor diffusion in the GDL, which is driven by the air input RH, and mass convection in the flow field, which is driven by air input flow rate. Potential flooding of the electrodes was assessed as a function of these two input conditions. The results of the two experiments were compared and a correlation was found between performance and water removal rates which, ultimately, provides valuable insight into water management in PEMFCs.

7.1 Summary of Findings

The main findings of this thesis are summarized below:

- There is a significant positive relationship between flow rate and performance.
- There is a significant negative relationship between RH and performance.
- There is a significant interaction between flow rate and RH, such that the positive effect of flow rate on performance is greatest at RH levels above 35%. There is only a slight increase in the power density output between the 35-3 and 35-6 conditions.
• The effect size of flow rate exceeds that of either RH or the FR × RH interaction, attesting to its importance for fuel cell performance.
• The highest performance was demonstrated by the 65-6 condition (i.e., an inlet air RH of 65% at the high flow rate), which obtains a power density of 0.470 W/cm².
• The low flow rate resulted in lower quasi in-situ capabilities of water removal across all conditions, except for at the highest humidity level of 125% RH, during which both flow rates obtained similar water removal rates.
• Higher quasi in-situ water removal capabilities were evident as RH decreased.
• There was a consistent water vapor diffusivity trend along the length of the flow channels during quasi in-situ testing, such that the sections near the inlet had a higher rate of water removal as compared to the sections near the outlet.
• Good in-situ performance is most likely to occur when the quasi in-situ water removal rates are greater than or equal to the water production rate at 1 A/cm². The 65-6 condition, which has a water removal rate that matched the production rate at 1 A/cm², achieves the highest in-situ performance results. The 35-3 and 35-6 conditions (i.e., an inlet air RH of 35% at the low and high flow rates, respectively) produce quasi in-situ removal rates that exceed the production rate at 1 A/cm² and obtain comparably high performance.
• The water vapor diffusion model produced strong validity and high predictability.
• The final effective water vapor diffusion coefficient of the studied GDL with an MPL is 0.0481 cm²/s at 70°C.
• Total water removal rates were consistent between the cathode air and quasi in-situ air for the low flow rate conditions; the cathode air obtained higher water removal rates than the quasi in-situ air for the high flow rate conditions.

• Since the low flow rate resulted in insufficient water removal, poor performance ensued. This outcome was attributed to high water content at the anode and resultant flooding of both electrodes. In contrast, since the high flow rate resulted in increased water removal for the in-situ cathode, good performance was achieved regardless of inlet air humidity level.

7.2 Contributions

The contributions that this study has made to the research field are outlined below:

• The novel segmented water plate utilized in the quasi in-situ component of this study extends our understanding of local water removal through the GDL along the length of the flow field, rather than being limited to the inlet and outlet properties.

• The segmenting method and analytical model employed in this study offer a precise tool to extract the effective water vapor diffusion coefficient of the GDL from the experimental results while accounting for mass convection in the channel.

• Several factors interact to affect in-situ performance, which makes it difficult to differentiate the effects of independent factors. Using the in-situ and quasi in-situ methods in parallel allows us to assess the isolated effect of the GDL and flow field on water management during PEMFC operation.

• The quasi in-situ experimental design allows water management aspects that are typically studied using ex-situ techniques to be examined under conditions that
approximate in-situ operation, which provides a more realistic representation of the mechanisms of water removal occurring in PEMFCs.

- The quasi in-situ setup has the capability to characterize a wide range of GDL/MPL, PEM, and MEA configurations across an array of test conditions.

### 7.3 Future Directions

Suggestions for future research directions are listed below:

- Test a wide range of GDLs using the experimental method outlined in this thesis to determine the impact of the GDL on water transport and performance.
- Add a PEM (proton exchange membrane) to the water side of the GDL and compare the results to those obtained with the GDL only, in order to quantify water transport in the PEM.
- Vary the type, shape, and dimensions’ of the flow field to examine how these aspects might alter water removal characteristics and impact fuel cell performance.
- Investigate the effect of cell temperature on quasi in-situ water removal rates and in-situ performance more thoroughly by testing a broader range of temperatures.
- Control/increase the pressure at the top of the water columns to study liquid phase permeation and the role of GDL/MPL capillary pressure on water transport.
- Induce a temperature gradient from the water to the air side and along the length of the flow channel for the quasi in-situ setup, to more closely mimic in-situ fuel cell operation (e.g., place a heating source on the water side that matches the heat flux generated in an operational fuel cell).
REFERENCES


doi:10.1016/j.electacta.2014.11.143


APPENDIX A: HUMID AIR PROPERTIES

Section A.1 covers the fundamental parameters of ideal gas mixtures and provide details about gas mixture properties, outlining these properties for an air and water vapor mixture (humid air). Section A.2 assesses the thermophysical and transport properties of humid air.

A.1 Fundamental Parameters

McQuiston, Parker, and Spitler (2005) [62] review the fundamental parameters of humid air. Dry atmospheric air is comprised of many constituents; 21% Oxygen, 78% Nitrogen, and 1% other (by volume). Humid air consists of a mixture of dry air and water vapor, where the water content ranges from dry air (no water vapor) to saturated air (no more water vapor can be held). All components of this gas mixture follow the ideal gas law (Equation A.1) (at pressures below three atmospheres).

\[ p_i = \rho_i R T \]  
\( \text{(A.1)} \)

Put in other terms, the density of a component can be found using Equation A.2.

\[ \rho_i = \frac{p_i}{R_i T} \]  
\( \text{(A.2)} \)

The gas constant for an individual component can be found using Equation A.3.

\[ R_i = \frac{\bar{R}}{M_i} \]  
\( \text{(A.3)} \)

The universal gas constant, \( \bar{R} \), is 8.314 \( \left[ \frac{J}{molK} \right] \), and the molecular mass of dry air and water vapor are:

\[ M_a = 0.0289635, \ M_v = 0.018015 \left[ \frac{kg}{mol} \right] \]
Therefore, the gas constants of dry air and water vapor are:

\[ R_a = 287.0509, \quad R_v = 461.5043 \frac{J}{kgK} \]

The Dalton law (Equation A.4) states that the pressure of a mixture of ideal gases is equal to the sum of the partial pressures of its constituents (i.e., dry air and water vapor for humid air).

\[ P = p_a + p_v \quad (A.4) \]

The mole fraction of each component is equal to the ratio of its partial pressure to the total pressure (Equation A.5).

\[ x_i = \frac{p_i}{P} \quad (A.5) \]

Saturated air occurs when the partial pressure of water vapor reaches the saturation vapor pressure of liquid water at the same temperature and pressure. At this state, an equilibrium state is formed between the water vapor in the humid air and liquid water. If any further water is added, the humid air will not absorb it as water vapor, instead it will remain in the liquid state.

The relative humidity (RH) of humid air (Equation A.6) is the ratio of the mole fraction of water vapor in a mixture to the mole fraction of water vapor in a saturated mixture (at the same temperature and pressure).

\[ \phi = \left[ \frac{x_v}{x_s} \right]_{i,p} \quad (A.6) \]

The RH can also be expressed using Equation A.7.

\[ \phi = \frac{p_v}{p_s} \quad (A.7) \]
The saturation vapor pressure, \( p_s \), as a function of temperature given by [62] may be found in Table A-1. Another correlation for the saturation vapor pressure given by Tsilingiris (2008) [61] is given in Equation A.8. Numerical constants for Equation A.8 are listed in Table A-2. The listed values in Table A-1 and the values found using Equation A.8 for the saturation vapor pressure of water are plotted in Figure A-1 as a function of temperature (from 0-100°C). The saturation pressure at 70°C is listed as 31180 Pa from Table A-1 [62], and is calculated as 29033 Pa using Equation A.8 [61]. For the purposes of this study, the values from Table A-1 are used for the water saturation vapor pressure.

\[
p_s = \left[ E_0 + E_1 \cdot t + E_2 \cdot t^2 + E_3 \cdot t^3 + E_4 \cdot t^4 \right] \cdot 10^3 \tag{A.8}
\]

The mole fraction of water vapor and dry air are given by Equation A.9.

\[
x_v = \frac{\phi p_v}{P}, \quad x_a = 1 - x_v \tag{A.9}
\]

The partial pressure of water vapor and dry air are given by Equation A.10.

\[
p_v = \phi p_s, \quad p_a = P - p_v \tag{A.10}
\]

The humidity ratio (Equation A.11) represents the ratio of the mass of water vapor to the mass of the dry air in the mixture.

\[
\omega = \frac{m_v}{m_a} \tag{A.11}
\]

Equation A.12 can be found by substituting the ideal gas law (Equation A.1) into Equation A.11.

\[
\omega = \frac{M_v p_v}{M_a p_a} \tag{A.12}
\]

The humidity ratio as a function of relative humidity, as well as saturation and total pressure (Equation A.13) can be found by combining Equations A.12 and A.10.
\[
\omega = \frac{0.6219 \phi p_s}{P - \phi p_s}
\]  \hspace{1cm} (A.13)

Equation A.14 can be found by rearranging Equation A.13, solving for relative humidity as a function of humidity ratio, as well as saturation and total pressure.

\[
\phi = \frac{P}{p_s \left(1 + \frac{0.6219}{\omega}\right)}
\]  \hspace{1cm} (A.14)

Since the humid air consist of multiple components, mixture properties of the ideal gas must be found. The total mass flowrate of the mixture is shown in Equations A.15 and A.16.

\[
\dot{m}_m = \dot{m}_u + \dot{m}_v
\]  \hspace{1cm} (A.15)

\[
\dot{m}_m = \dot{m}_u + \omega \dot{m}_a
\]  \hspace{1cm} (A.16)

Table A-1. Saturation vapor pressure as a function of temperature [62]

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Pressure (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>610</td>
</tr>
<tr>
<td>5</td>
<td>870</td>
</tr>
<tr>
<td>10</td>
<td>1230</td>
</tr>
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<td>84530</td>
</tr>
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<td>101320</td>
</tr>
</tbody>
</table>
Figure A-1. Plot of saturation vapor pressure of water as a function of temperature

The mass fraction of each component is equal to the ratio of its mass flow rate to the mixture mass flow rate (Equation A.17).

\[ \dot{m}_{f,i} = \frac{\dot{m}_i}{\dot{m}_m} \]  

(A.17)

The specific enthalpy of humid air is the sum of the enthalpies of dry air and water vapor, as shown in Equation A.18.

\[ i_m = i_a + \omega \cdot i_v \]  

(A.18)

The enthalpy of dry air and water vapor are given by Equations A.19 and A.20, respectively.

\[ i_a = c_{p,a} t \]  

(A.19)

\[ i_v = i_g + c_{p,v} t \]  

(A.20)

Therefore, the specific enthalpy of humid air is shown in Equation A.21.
Assuming the specific heat capacities remain constant at \( c_{p,a} = 1.0 \) and \( c_{p,v} = 1.86 \ \text{kJ/(kg} \cdot \text{°C)} \), and the enthalpy of saturated water vapor at 0 °C is \( i_g = 2501.3 \ \text{kJ/kg} \), [62] reports Equation A.22 for evaluating the enthalpy of humid air.

\[
i_m = c_{p,a} t + \omega \left( i_g + c_{p,v} t \right)
\]  \hspace{1cm} (A.21)

When the humid air reaches 100% relative humidity (saturated humid air), any further water will be in a liquid state. The enthalpy of the liquid water (Equation A.23) may be added to the enthalpy of saturated air, to find the total enthalpy shown in Equation A.24.

\[
i_w = c_{p,w} t
\]  \hspace{1cm} (A.23)

\[
i_m = c_{p,a} t + \omega \left( i_g + c_{p,v} t \right) + \left( \omega - \omega_s \right) c_{p,w} t
\]  \hspace{1cm} (A.24)

Assuming the specific heat capacity of water remains constant at \( c_{p,w} = 4.186 \ \text{kJ/(kg} \cdot \text{°C)} \), the total enthalpy of over-saturated air is given in Equation A.25.

\[
i_m = \left[ 1.0t + \omega_s \left( 2501.3 + 1.86t \right) \right] \cdot 10^3
\]  \hspace{1cm} (A.25)

The saturation humidity ratio, \( \omega_s \), is found by evaluating Equation A.13 at \( \phi = 1 \), and the total humidity ratio, \( \omega \), represents the total water content (water and vapor) per unit mass of dry air.

### A.2 Thermophysical and Transport Properties

This section outlines the correlations given by Tsilingiris (2008) [61] for the thermophysical and transport properties for humid air as a function of temperature and relative humidity. All of the results found by the author are in good agreement with results reported by other literature [3, 25].
Gas constant

The gas constant for the mixture is the ratio of the universal gas constant to the mixture molecular mass (Equation A.26).

\[ R_m = \frac{\bar{R}}{M_m} \] (A.26)

The molecular mass, \( M_m \), of the mixture is found using Equation A.27.

\[ M_m = \frac{1}{\sum \left( \frac{m_{f,i}}{M_i} \right)} = \sum (x_i M_i) \] (A.27)

Therefore, the mixture gas constant for humid air can be solved using Equation A.28.

\[ R_m = \sum (m_{f,i} R_i) = m_{f,a} R_a + m_{f,v} R_v \] (A.28)

Density

The density of the mixture is given in Equation A.29.

\[ \rho_m = \frac{P}{R_m T} \] (A.29)

Viscosity

The dynamic viscosity of humid air can be found using Equation A.30. The mole fraction was given in Equation A.9 as \( x_v = \frac{\phi p_v}{P} \).

\[ \mu_m = \frac{(1-x_v) \mu_a}{(1-x_v) + x_v \Phi_{av}} + \frac{x_v \mu_v}{x_v + (1-x_v) \Phi_{wv}} \] (A.30)

In the above equation, the interaction parameters for dynamic viscosity are:
The dynamic viscosity of dry air can be found using Equation A.31.

\[ \mu_a = \left[ M_{A_0} + M_{A_1} \cdot T + M_{A_2} \cdot T^2 + M_{A_3} \cdot T^3 + M_{A_4} \cdot T^4 \right] \cdot 10^{-6} \] (A.31)

The dynamic viscosity of water vapor can be found using Equation A.32.

\[ \mu_v = \left[ M_{V_0} + M_{V_1} \cdot t \right] \cdot 10^{-7} \] (A.32)

Numerical constants for Equations A.31 and A.32 are listed in Table A-2.

The kinematic viscosity of the humid air is the ratio of the mixture dynamic viscosity to the mixture density (Equation A.33).

\[ \nu_m = \frac{\mu_m}{\rho_m} \] (A.33)

**Thermal Conductivity**

In a similar fashion to the viscosity, the thermal conductivity of humid air can be found using Equation A.34.

\[ k_m = \frac{(1-x_v)k_a}{(1-x_v) + x_v \Phi_{av}} + \frac{x_v k_v}{x_v + (1-x_v) \Phi_{va}} \] (A.34)

The interaction parameters for thermal conductivity are:

\[ \Phi_{av} = \frac{\sqrt{2}}{4} \left( 1 + \frac{M_a}{M_v} \right)^{1/2} \left[ 1 + \left( \frac{k_a}{k_v} \right)^{1/2} \left( \frac{M_v}{M_a} \right)^{1/4} \right]^2 \]
\[ \Phi_{\text{w}} = \frac{\sqrt{2}}{4} \left( 1 + \frac{M_v}{M_a} \right)^{-\frac{1}{2}} \cdot \left[ 1 + \left( \frac{k_v}{k_a} \right)^{\frac{1}{2}} \cdot \left( \frac{M_a}{M_v} \right)^{\frac{1}{4}} \right]^2 \]

The thermal conductivity of dry air can be found using Equation A.35.

\[ k_a = \left[ K A_0 + K A_1 \cdot T + K A_2 \cdot T^2 + K A_3 \cdot T^3 + K A_4 \cdot T^4 + K A_5 \cdot T^5 \right] \cdot 10^0 \quad (A.35) \]

The thermal conductivity of water vapor can be found using Equation A.36.

\[ k_v = \left[ K V_0 + K V_1 \cdot t + K V_2 \cdot t^2 \right] \cdot 10^{-3} \quad (A.36) \]

Numerical constants for Equations A.35 and A.36 are listed in Table A-2.

**Specific heat capacity**

The specific heat capacity of the mixture can be found using Equation A.37.

\[ c_{p,m} = \sum \left( m_{f,i} c_{p,i} \right) = m_{f,a} c_{p,a} + m_{f,v} c_{p,v} \quad (A.37) \]

The specific heat capacity of dry air can be found using Equation A.38.

\[ c_{p,a} = \left[ C A_0 + C A_1 \cdot T + C A_2 \cdot T^2 + C A_3 \cdot T^3 + C A_4 \cdot T^4 \right] \cdot 10^3 \quad (A.38) \]

The specific heat capacity of water vapor can be found using Equation A.39.

\[ c_{p,v} = \left[ C V_0 + C V_1 \cdot t + C V_2 \cdot t^2 \right] \cdot 10^3 \quad (A.39) \]

Numerical constants for Equations A.38 and A.39 are listed in Table A-2.

**Thermal diffusivity**

The thermal diffusivity (Equation A.40) represents the ratio of the thermal conductivity to the heat capacity. The thermal diffusivity for humid air can be found by substituting Equations A.29, A.34, and A.37 for density, thermal conductivity, and specific heat capacity for humid air, respectively, in Equation A.40.
\[ \alpha_m = \frac{k_m}{\rho_m c_{p.m}} \]  

**Prandtl number**

The Prandtl number is defined as the ratio of momentum to thermal diffusivity. The Prandtl number for humid air (Equation A.41) can be found by substituting Equations A.30, A.34, and A.37 for dynamic viscosity, thermal conductivity, and specific heat capacity for humid air, respectively, in Equation A.41.

\[ Pr_m = \frac{v_m}{\alpha_m} = \frac{\mu_m c_{p.m}}{k_m} \]  

**Mass diffusivity**

The binary mass diffusion coefficient for water vapor in air at one atmosphere can be estimated from the relation given in Equation A.42, reported by [25].

\[ D_{v,a} = \frac{0.26 \cdot 10^{-4}}{298^{\frac{3}{2}}} \cdot T^{\frac{3}{2}} \]  

Another correlation for the water vapor diffusion coefficient at one atmosphere reported by Nellis and Klein (2008) [64], derived using the Chapman and Enskog relationship, is given in Equation A.43. Numerical constants for Equation A.43 are listed in Table A-2.

\[ D_{v,a} = DAV_0 + DAV_1 \cdot T + DAV_2 \cdot T^2 \]  

The values found using Equations A.42 and A.43 are plotted in Figure A-2. The mass diffusivity for water vapor in air at 70°C is 0.321 cm²/s, using both Equations A.42 and A.43. For the purposes of this study, the diffusion coefficient for water vapor in air is found using Equation A.42.
Figure A-2. Plot of mass diffusivity of water vapor in air as a function of temperature

**Schmidt number**

The Schmidt number is defined as the ratio of momentum and mass diffusivity. The Schmidt number for humid air (Equation A.44) can be found substituting Equations A.29, A.30, and A.42 for density, dynamic viscosity, and mass diffusivity for humid air, respectively, in Equation A.44.

\[
Sc_m = \frac{v_m}{D_{v,a}} = \frac{\mu_m}{\rho_m D_{v,a}} \quad (A.44)
\]

**Lewis number**

The Lewis number is defined as the ratio of thermal and mass diffusivities. The Lewis number for humid air (Equation A.45) can be found by substitution Equations A.41 and A.44 for Prandtl number and Schmidt number, respectively, in Equation A.45.

\[
Le_m = \frac{\alpha_m}{D_{v,a}} = \frac{Sc_m}{Pr_m} \quad (A.45)
\]
<table>
<thead>
<tr>
<th>Eq.</th>
<th>Property</th>
<th>Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.8*</td>
<td>( p_x )</td>
<td>( E_0 = 0.7073034146 \times 10^0 )</td>
</tr>
<tr>
<td>A.31*</td>
<td>( \mu_\alpha )</td>
<td>( MA_0 = -9.8601 \times 10^{-1} )</td>
</tr>
<tr>
<td>A.32*</td>
<td>( \mu_v )</td>
<td>( MV_0 = 8.058131868 \times 10^1 )</td>
</tr>
<tr>
<td>A.35*</td>
<td>( k_\alpha )</td>
<td>( KA_0 = -0.276501 \times 10^{-3} )</td>
</tr>
<tr>
<td>A.36*</td>
<td>( k_v )</td>
<td>( KV_0 = 1.761758242 \times 10^1 )</td>
</tr>
<tr>
<td>A.38*</td>
<td>( c_{p,v} )</td>
<td>( CA_0 = 0.103409 \times 10^1 )</td>
</tr>
<tr>
<td>A.39*</td>
<td>( D_{a,v} )</td>
<td>( DA_0 = 1.86910989 \times 10^9 )</td>
</tr>
<tr>
<td>A.43**</td>
<td>( D_{a,v} )</td>
<td>( DAV_0 = -2.775 \times 10^6 )</td>
</tr>
</tbody>
</table>

**Note.** *Tsilingiris (2008) [61]. **Nellis and Klein (2008) [64]. All equations are valid in the range of 0-100°C.
Summary of final properties

Table A-3 lists the main thermophysical and transport properties of humid air at 70°C and an atmospheric pressure of 101325 Pa (as these are the main temperature and pressure for the study) from dry air to saturated air ($\phi = 0 \rightarrow 1$).

Table A-3. Thermophysical mixture properties of humid air at 70°C and 101325 Pa as a function of relative humidity

<table>
<thead>
<tr>
<th>RH (%)</th>
<th>$\rho_m$</th>
<th>$\mu_m (\cdot 10^6)$</th>
<th>$k_m (\cdot 10^{-3})$</th>
<th>$Pr$</th>
<th>$Sc$</th>
<th>$Le$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.0287</td>
<td>20.5069</td>
<td>29.1614</td>
<td>0.7101</td>
<td>0.6205</td>
<td>0.8739</td>
</tr>
<tr>
<td>5</td>
<td>1.0227</td>
<td>20.3483</td>
<td>29.0762</td>
<td>0.7130</td>
<td>0.6193</td>
<td>0.8686</td>
</tr>
<tr>
<td>35</td>
<td>0.9868</td>
<td>19.4037</td>
<td>28.5538</td>
<td>0.7306</td>
<td>0.6120</td>
<td>0.8377</td>
</tr>
<tr>
<td>65</td>
<td>0.9509</td>
<td>18.4711</td>
<td>28.0112</td>
<td>0.7490</td>
<td>0.6046</td>
<td>0.8073</td>
</tr>
<tr>
<td>95</td>
<td>0.9150</td>
<td>17.5502</td>
<td>27.4477</td>
<td>0.7680</td>
<td>0.5970</td>
<td>0.7773</td>
</tr>
<tr>
<td>100</td>
<td>0.9090</td>
<td>17.3979</td>
<td>27.3516</td>
<td>0.7713</td>
<td>0.5957</td>
<td>0.7724</td>
</tr>
</tbody>
</table>