Cathode Pressure Modeling of the Buckeye Bullet II 500kW PEM Fuel Cell System

Dissertation

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ABSTRACT

This dissertation details the development of a model that simulates the pressure dynamics of the cathode supply system for the Buckeye Bullet 2, the world’s fastest hydrogen fuel cell vehicle. Due to the extreme power levels of the BB2 system, and the unique use of heliox as the oxidant supply, it is shown that existing system level models for predicting the fuel cell pressure dynamics do not adequately capture the dynamics of the BB2 system. Several modeling attempts are evaluated, and eventually the most robust model is a model which is derived from a rational system decomposition of the cathode system. By separating the major losses of the cathode system into an upstream and downstream resistance, the performance of the model is significantly improved. It is shown that the rate at which water exits the cathode plays a significant role accurately capturing the pressure dynamics. With this in mind, a distributed parameter model is developed to provide estimates of how the rate of liquid water removal from cathode changes with time. The results of this model are validated through physical testing. The resulting model relies on five empirically tunable parameters to tune the model performance to match that of the system. The method of calibrating these parameters is outlined, and the resulting model developed with stationary test data is compared to data from the actual BB2 race data. Only a few parameters need to be recalibrated, which is due to physical system differences between the data from the stationary tests and the race data.
Dedicated to outstanding members of the Buckeye Bullet team, past, present, and future.
ACKNOWLEDGMENTS

To say this work is the result of standing on the shoulders of giants, is an understatement when talking about the members of the Buckeye Bullet team. Their selfless dedication to the program for over 10 years has allowed the first doctoral work from the program to be completed, after 8 masters works to date. Seeing the program grow from its early years, where parts were designed around the pieces available at the local metal scrap yard, to a professional level race team, interacting with major companies from all over the world, has been an amazing development to witness. I am grateful to have been a part of it.

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CHAPTER 1

INTRODUCTION

On September 25th, 2009, the Buckeye Bullet 2 became the first hydrogen fuel-cell vehicle to eclipse the 300 MPH mark, setting an international speed record of 302.877 MPH in the flying mile. The Buckeye Bullet 2 program included over 2 years of initial conceptual design, followed by 3 years of testing, racing, and development. This dissertation details the development of a system model used to simulate the cathode pressure dynamics of the most powerful vehicular fuel cell system ever developed.

1.1 Electric Racing at Ohio State

2009 marked the 15th anniversary of Ohio State’s involvement in electric racing. Ohio State has been involved in three separate electric racing endeavors, the Smokin’ Buckeye, the Buckeye Bullet, and the Buckeye Bullet 2.

1.1.1 The Smokin’ Buckeye

The Smokin’ Buckeye is an electric race vehicle that participated in the Formula Lightning Series. OSU campaigned the Smokin’ Buckeye from 1994 to 2002. The racing series was a collegiate open wheel formula style race that traveled to major
racetracks around the country. Thirty-one lead acid batteries powered an AC induction traction system capable of race track speeds over 120 mph. The team could do a pit stop with a full battery change in under 17 seconds. Ohio State dominated the competition winning more than 50% of the races entered and every national championship ever awarded. The vehicle was retired from competition in 2002.

Figure 1.1: The Ohio State University Smokin’ Buckeye

1.1.2 The OSU Land Speed Racing Program

The Buckeye Bullet program began as the Formula Lightning series was ending. The program pushes electric traction technology to its limits through the ultimate test of vehicle engineering, land speed racing. Land speed racing allows vehicles to be pushed to their top speed, while racing against the clock for the simple glory of achieving a speed record in their class. Ohio State has been working on land speed racing since 2001, and has built two distinct vehicles that hold land speed records, the Buckeye Bullet 1 (BB1), and the Buckeye Bullet 2 (BB2).
Land Speed Racing

A vehicle may set either a U.S. land speed record, or an international land speed record. Fig. 1.2 graphically shows the difference between the two records.

US land speed records are certified by the SCTA-BNI. These records are set on a seven mile course, and are run at the Bonneville Salt Flats in the Utah. The vehicle accelerates over the first two miles. The vehicle is timed over the middle three miles. If the fastest average speed over one of these miles exceeds the standing record in the class, the vehicle is sent to impound. The team then has up to four hours to service the vehicle. Depending on the time of day, the vehicle may run again that
same day, or wait until the following day. If the return run is made the following day, the team is allowed another hour to prepare the vehicle in the morning. The vehicle will then run on the same course, in the same direction, and again be timed over the middle three miles. The average speed from the two runs is used to determine the new speed record.

International speed records are certified by the FIA. These records may be set on any length course. Recently in the US these records have been run at The Bonneville Salt Flats on an 11 mile course. The vehicle is timed over a middle mile and middle kilometer. Once the vehicle enters the timed portion of the course, it must complete a return run through the timed section, in the opposite direction, within one hour. The average of the two runs is used to set the record for the average speed in the flying mile and flying kilometer.

1.1.3 The Buckeye Bullet 1

The BB1 is a battery powered vehicle that was designed to break the land speed record for electric vehicles, which was previously 245 mph, set by the White Lightning in 1999. The BB1 debuted on the Bonneville salt flats in October of 2002. Over the course of 3 years of racing and optimization, the BB1 worked its way up to a peak speed of 321 mph. October of 2004 saw the top record speeds of the BB1 and the shattering of the existing records. The new U.S. record was set at 314.958 mph. The BB1 was retired after its October 2004 runs, but still holds the U.S. land speed record in the E/III class (Electric power, over 1000 kg).

The BB1 also set an unofficial international record speed of 271.737 mph. This record is not an official FIA record, because the FIA was not present to certify the
record in 2004. Instead it was certified by the SCTA-BNI, and was set under the rules established by the FIA. The difference between the BB1 international and US record speeds is because the BB1 team could only afford a single battery pack. The extreme nature of the race meant that the batteries could not handle a full power run, a full recharge, and another full power run all within one hour. Thus the team was forced to run the vehicle with reduced power to avoid damaging the battery pack.

The BB1 program was very successful. After the 2004 race season the team decided to retire the BB1 and look for a technology that would enable them to set an FIA record over 300 MPH. Fuel cell vehicles can be refueled with hydrogen very quickly, so the team set their sites on building a hydrogen fuel cell vehicle.

1.1.4 Buckeye Bullet 2

The goal of the BB2 was to break the existing records for hydrogen fuel cell vehicles, as well as break the speeds achieved by the BB1, and set an FIA record for electric traction vehicles over 300 MPH. The BB2 uses the same motor and inverter used in the BB1, but places them in an entirely new vehicle that can be seen in Fig. 1.4.

Fuel cells are used in the BB2 to provide the DC electricity to the inverter, instead of the batteries in the BB1. The fuel cells are provided by Ballard Power Systems, of
Burnaby, BC, Canada. The fuel cells are packaged in two separate fuel cell modules (FCMs). Two FCMs of this construction were originally used by Ballard as part of a worldwide hydrogen fuel cell bus demonstration program[1, 2]. The maximum power of the two FCMs was 250 kW in the original design configuration for the city buses. To provide the required power for the BB2, the fuel cell power was increased to over 500 kW.

To develop this kind of power from a fuel cell, many unique supply systems were developed. A typical fuel cell system requires a controlled supply of Hydrogen, Oxygen, and Coolant. These system details are provided in Chapter 3.
1.2 Motivation

The motivation for this dissertation first comes from its application specifically to the BB2 vehicle, and is further supported by the current needs of the fuel cell industry.

1.2.1 Motivation Related to the Buckeye Bullet

The first part of the motivation for this dissertation comes from the desire to maximize fuel cell power for the purpose of achieving the BB2 record speeds. Generating over 500 kW of power from a fuel cell system designed for 250 kW requires the ability to push all components of the system to their design limits. Through the testing and development, and early racing of the BB2, several problems were found with the pressure control of the cathode supply system.

Maximum fuel cell power can always be achieved when operating pressure is maximized. However, attention must be paid to not exceed the pressure limitations of the components in the system. Among the most sensitive components of the system are the seals of the fuel cell stack. In the first two years of the BB2 program the stack seals failed twice due to excess cathode pressure. This is a highly dangerous condition where a failed seal on the stack can lead to the leakage of fuel and oxidant gases. When these two gases mix they become highly flammable, and hence a dangerous mixture. In addition, hydrogen flames are not visible to the human eye.

If a robust and reliable fuel cell model were available to model the pressure conditions of this fuel cell system, then system design and control would be far easier. The problem is that simple models, and even the most commonly available system models do not very accurately capture the dynamics of the BB2 system. The
BB2 provides an opportunity to develop a new model for the BB2’s uniques system, and the knowledge gained from its development should be applicable to a standard fuel cell system.

1.2.2 Motivation Related to the Status of Fuel Cell System Design

Further motivation comes from the current status of fuel cell development. During the development of the Ballard bus FCMs (circa 2000), Ballard designed the FCM, and all its associated supply systems. They acted as the stack designer, the system designer, and the system integrator. Similar development was also the trend in automotive fuel cell development, as well as for other applications such as stationary power or fork lifts.

Recently the trend of a single company completing stack design, system design, and system integration has changed dramatically. Some fuel cell stack designers have decided to focus all their resources on the design, development, and cost reduction of the core component, the fuel cell stack. This means that separate companies are now responsible for the design of the systems, and sometimes a third company is responsible for total system integration.

This trend in the joint development of a fuel cell vehicle leads to the need for models that can be shared between the various parties involved. The stack manufacturers may have very detailed models of the stack and its performance, but they may be unwilling to share these models due to their proprietary nature. The other problem is that these models may be far too complicated and too computationally complex to be used in control development of the fuel cell systems. A robust system level model that can be exchanged between the stack manufacturer, and the system
integrator would be very useful to aid in the rapid design, and robust control of the complete system.

1.3 Dissertation Objectives

The objective of this dissertation is to develop a robust system model that can be used to model the pressure dynamics of the BB2 system. This model will be validated through the vast amount of test data that is available from the BB2 race vehicle.

The model should be of a structure that would allow its principles, and empirically derived elements to be applied to a variety of more common fuel cell systems. This dissertation model development will fill a gap in the current literature for the development of a control oriented fuel cell system model that considers liquid water production.

An empirically tunable control oriented model of this nature would be very useful to system integrators. They may not have access to the detailed models used by the stack designers, or these models may be too complex for doing system design and simulations. Hopefully a model of this nature would be provided by the stack manufacturer for use by the system integrator, but if it were not, the integrator may be able to conduct testing to create such a model.

1.4 Contributions of this Dissertation

This dissertation is unique in several ways. First the dissertation is based around a completely unique fuel cell system. The BB2 fuel cell system is arguably the most powerful automotive PEM fuel cell system ever developed. The doubling of power
output relative to the original system design means that this dissertation examines the extreme limits of fuel cell system performance.

This dissertation presents test data that is the result of years of development and testing and tuning to achieve reliable system performance from the system that supplies the BB2. Details are provided in this dissertation about the system testing and tuning that was required to enable the system to operate properly so the data can even be analyzed. The design and testing of these systems is a major portion of the work involved in the presentation of this work.

The extreme power levels of the system allow a unique opportunity to record measurable water outlet flow rates from a fuel cell system. Often very complicated tests are require to measure the trace amounts of water produced from single cells. The ability to capture this water and correlate its output rate to a simplified model is truly unique.

This work is also unique in its development of a simplified model to predict the outlet flow rate of water. Most studies involving two-phase flow deal with very detailed single cell models, and don’t pay attention to the dynamics of the entire system. This work applies a simple model to explain a very complex behavior and shows some very good success.

This work is unique in its inspection of the pressure dynamics of the cathode system, and especially how they relate to the liquid water. One of the most commonly referenced models in the literature completely ignores the liquid water production.

This work is also unique in its three step approach to modeling the pressure dynamics of the cathode. Using a rational system decomposition, the model uses one resistance up stream of the cathode, that deals only with single phase flow. The
model uses a second model that is able to predict the water outlet flow rate of the cathode, and then adds a 3rd model that provides a variable resistance that changes based on the water outlet flow rate.

In summary this work is unique in its path toward developing and validating a simplified model capable of predicting the pressure dynamics of arguably the most powerful vehicular fuel cell system ever.

1.5 Dissertation Organization

Chapter 2 provides a simple introduction into the basic operation of fuel cells, and provides some information on their use in automotive transportation. The chapter then provides a review of the many ways in which fuel cells can be modeled, from detailed 1D computational models, to 3D CFD models, and the very few existing control level models.

Chapter 3 first gives a more detailed account of the specific design of the BB2 fuel cell systems. The chapter then provides the details of the models that have been developed for use in the simulation of the BB2 fuel cell system performance.

Chapter 4 provides the details on the experimental methods used for the BB2. The chapter also gives many of the details of the tuning, and performance optimization that was required for the fuel cell system to reliably provide over 500 kW of power.

Chapter 5 provides a detailed look at the results of the modeling applied to the BB2 system. It begins by showing the results of the most commonly available control oriented fuel cell system model when applied to the BB2. The results are shown to have several shortcomings. The chapter then shows the results of several
models that are used to improve the modeled performance of the system. The final model presented is chosen as the best model, and details on the calibration of that model are presented.
CHAPTER 2

LITERATURE REVIEW

This chapter provides a basic background on fuel cells, and details the most relevant models and research used in fuel cell modeling. The concept of a fuel cell, from its basic operation, to its integration into a full stack is detailed first. Because of the automotive nature of the BB2 system, some information on fuel cells for general automotive use is also provided. Finally the chapter provides a literature review of the various aspects of fuel cell modeling. Fuel cell modeling can begin with single cell 1D models, and progress to complicated 3D models. Very few models are intended for dealing with two-phase flow. A limited number of system models have been developed, and none of the system models deal with liquid water production.

2.1 Basic Fuel Cell Principles

A fuel cell is an electrochemical device that converts chemical energy into electricity. Several different types of fuel cells exist, with common types including PEM, Alkaline, and SOFC. For the case of the BB2, a hydrogen PEM fuel cell is used. In a hydrogen fuel cell, hydrogen and oxygen are reacted to form water. Through the fuel cell reaction useful electricity is generated. The basic operating principle of the fuel cell can be seen in Fig. 2.1.
Figure 2.1: Fuel Cell Basic Operation [3]
The single cell is constructed of an anode and a cathode separated by a polymer electrolyte membrane. Hydrogen is supplied to the anode and oxygen is supplied to the cathode. At the anode, the hydrogen gas ionizes forming electrons and protons. The electrolyte membrane carries the proton to the cathode. An external circuit carries the electron to the cathode to complete the reaction according to equations 2.1, 2.2, and 2.3. The Polymer Electrolyte Membrane (PEM) is the source of the term PEM, which is the most common way to refer to this type of fuel cell. PEM can also be an abbreviation for Proton Exchange Membrane, which is an equally accurate description.

\[
2H_2 + O_2 \rightarrow H_2O \tag{2.1}
\]

\[
2H_2 \rightarrow 4H^+ + 4e^- \tag{2.2}
\]

\[
O_2 + 4e^- + 4H^+ \rightarrow 2H_2O \tag{2.3}
\]

In a fuel cell, the relationship between the current draw, and the voltage available, is defined by the fuel cell’s polarization curve. The polarization curve is dominated by 3 areas of losses. Activation losses are present at low currents, and are dominated by the reaction kinetics, primarily on the cathode side. The next major area of loss is the ohmic loss region. The ohmic losses are generally proportional to current, and come from the resistance of the cells electrolyte to the conduction of protons. The final region of loss comes from the concentration losses. Concentration losses occur under high current draws, where the gas concentrations are depleted near the reaction sites, lowering the effective concentration of the gases to the point where the reaction cannot be sustained. A sample polarization curve highlighting these regions can be seen in Fig. 2.2.
The power available from a fuel cell is defined by its power curve, which is calculated directly from the polarization curve. Since electrical power is the product of voltage and current, the power can be plotted vs current. Figure 2.3 shows a sample power curve for a fuel cell. From the power curve, it is clear that to attain peak power, the fuel cell should be operated at higher current levels just before concentration losses take effect and reduce the power.

The hydrogen and oxygen must pass through a conductive gas diffusion electrode to reach the catalyst where the fuel is oxidized. At high currents, the partial pressure of oxygen at the fuel cell catalyst is limited by the rate of diffusion between the gas delivery channels and the catalyst. The lowered oxygen partial pressure reduces the fuel cell performance. The rate of diffusion $J$, is governed by Fick’s law.

\[
J = \frac{D_{eff}}{\Delta Z} \Delta \phi_{O_2} \tag{2.4}
\]
The diffusion coefficient, $D_{eff}$, can be increased by changing the balance gasses in the oxidant supply. In the BB2, a mixture of oxygen and helium is used to increase the diffusion coefficient. This increases the delivery rate of oxygen to the catalyst where it reacts with protons and electrons to complete the reaction.

2.1.1 Fuel Cells to Fuel Cell Stacks

The information in Section 2.1 details the operation of a single cell. A single cell will have an operating voltage of around 1 Volt DC, and the amount of current it can produce will be proportional to the surface area of the cell. Most applications, from stationary power generation, to fork lift applications, to automobiles, will require a much higher voltage output to interface with typical systems. For automotive use the industry trend is typically around 300V DC. In the specific case of the BB2, the required operating range for the inverter is between 600 V and 900 V DC.
To achieve the operating voltages that are required, the individual fuel cells can be combined in series, as shown in Fig. 2.4. Since the most common design of fuel cells is a prismatic shape, the anode bipolar plate from one cell, can be used as the cathode bipolar plate for the next cell in series. In this method, the prismatic cell are "stacked" onto each other, leading to the commonly used term of a fuel cell stack. A compressed stack is shown in Fig. 2.5.

2.2 Fuel Cells for Automotive Use

The PEM fuel cell is commonly regarded as the most promising fuel cell technology for future use in transportation systems. This is due to its lower operating temperature relative to fuel cells such as a Solid Oxide Fuel Cell (SOFC). Modern PEM fuel cells typically operate around 80 °C, while a SOFC may operate closer to
800 °C. The lower operating temperature is a key since personal automobiles require a quick start up time, and may be used for short trips. Therefore simply having a lower operating temperature reduces the time required for warm up.

Fuel cell vehicles hold great promise for the future, but there are still some technological hurdles to overcome. Fuel cells have long been targeted to replace the gasoline powered vehicles that we drive today.

To replace a gasoline vehicle, a fuel cell vehicle needs to be cost-competitive, have a similar life span (100,000 + miles, or about 5000 hours for the fuel cell), provide equal acceleration and driving performance, have a long driving range (300 + miles), operate in a wide variety of hot and cold environments, and have a useful network of refueling stations similar to gasoline. Progress is being made in each area.
Figure 2.6: Cost of an 80kW stack, past, present, and future goal [8].

Fuel cell costs have dropped remarkably since 2001. A Department Of Energy (DOE) report [5, 6] shows that costs have dropped from $275/kW in 2001 to $61/kW in 2009, and are projected to meet the DOE target $30/kW by 2015. Toyota has publicly announced they expect to have cost competitive fuel cell vehicles available by 2015[7].

Durability remains a key hurdle to overcome, with the 2008 DOE status being 1900 hours, with a 2015 goal of 5000 hours. The primary component that is being improved is the Membrane Electrode Assembly (MEA). The MEA contains expensive platinum that is used as a catalyst to facilitate the chemical reaction. Through improved materials, and a better understanding of the factors that lead to aging and degradation of the MEA, improvements in overall durability are being made.

Fuel cells originally were not able to be started in temperatures below freezing due to the production of water in the cell which would freeze the fuel cell. Design
and material changes to the fuel cell stack have solved the problem, and many manufacturers have demonstrated fuel cell vehicles that can be started at temperatures as low as -34 °C.

Fuel cells are easily able to provide enough power to make a vehicle accelerate and perform similar to a gasoline vehicle (as proven by the BB2). A battery system can be added to a gasoline engine vehicle to create a hybrid vehicle that uses less fuel, and drives further on a single tank. The same benefits can be seen by hybridizing a fuel cell vehicle which can create fuel cell vehicles with ranges of 400+ miles on a single tank, and have zero emissions from the vehicle.

The largest challenge is the refueling network. Hydrogen refueling stations will not be created until there is sufficient demand from owners of hydrogen vehicles, but demand for hydrogen fuel cell vehicles will remain low until consumers have a suitable network of stations. The burden to solve the problem falls on the vehicle manufactures who must show the technology is practical for use by the public, so a suitable network of stations can be built.

Progress is also being made in the development of high temperature PEM fuel cells. This may seem to counter act the benefit that a PEM fuel cell has over other fuel cells, however it simply refers to fuel cells that operate above 100 °C. Early membrane materials were not able to handle operation at these temperatures, or were only able to operate for very short life spans. However advances in the membrane materials have lead to new materials that allow high temperature operation [6].

Operating over 100 °C will provide PEM fuel cells with several benefits. The largest benefit will be the elimination of liquid water formation, since all product
water will be formed in the vapor state. In fact, one of the largest reasons for the work of this dissertation revolves around the problem of dealing with both liquid and vapor product water. High temperature operation will also significantly ease the humidification requirements of the system, leading to reduced system cost. A third benefit is found in the cooling requirements of a high temperature fuel cell. With a higher normal operating temperature, the required size of cooling system components such as automotive radiators, becomes reduced because there is a higher $\Delta T$ between the coolant and the ambient air, especially in hot environments.

From their beginning, hydrogen fuel cell vehicles have been tasked to match or outperform combustion engine vehicles in every aspect. Battery vehicles may have a greater chance of near term success due to their simplicity, but they require drivers to make sacrifices from what their vehicles currently provide in terms of range, size, and recharge time. It is most likely that the zero-emissions future will contain a combination of fuel cell and battery vehicles to meet the variety of needs of the driving public.

### 2.3 Unit Cell Modeling

The modeling of fuel cells can be a complex undertaking. Since the late 1980’s many forms of fuel cell modeling have been proposed. For the most part the modeling efforts are focused on creating models with the ability to predict the performance or operating condition of a single unit cell. The modeling can be relatively easily broken down into empirical or steady state models, simplified 1D models, and more complex 2D and 3D models that require CFD type solvers.
2.3.1 Empirical and Steady State Models

A very simple model can be quickly built if it is assumed the fuel cell is operating in a steady state condition, with optimized supply of reactants. If these conditions are true, then the simple polarization curve shown in Fig 2.2 is an excellent method of providing the basic characteristics of the fuel cell. If an operating current is the known input, then the operating voltage is directly calculated as the output. This is a fuel cell model in its simplest form.

Unfortunately, a polarization curve can only be created from a single set of operating conditions. Under steady state conditions, there will be a unique polarization curve for each and every combination of operating pressure, temperature, and reactant humidity, and reactant flow rate. It would theoretically be possible to test a fuel cell under a wider array of operating conditions, and use a set of maps and interpolate to generate a set of polarization curves for all operating conditions.

A better method is to apply a mechanistic method of creating a model, and then empirically calibrate the parameters of the model. This method has been used extensively by Amphlette et al. [9, 10, 11, 12]. This group starts by developing a mechanistic model of a fuel cell. This creates a set of algebraic expressions for the thermodynamic equilibrium potential, along with activation, ohmic, and mass transport losses. Based on this mechanistic model, numerical parametric equations for the voltage loss terms were determined from the empirical data. This same group has further extended the model to be used for transient behavior [13], to incorporate voltage degradation due to aging [14], and to include the anode activation losses [15], which are typically ignored in fuel cell modeling.
This method has been used for the analysis of the BB2, and was used both by Sinsheimer[16] and Bork[17] to aid in the development of the BB2 fuel cell system. Sinsheimer used empirical data from the first year of the BB2 to develop polarization curves that aided in the speed performance modeling of the BB2. During the second year of the program, many improvements to the fuel cell system were made, and Bork was able to use this model to show the improved performance of the fuel cell relative to the data that was available for Sinsheimer[17].

2.3.2 1D Models

To model a unit cell in one dimension, it is usually simplified as a single straight channel of uniform dimension. The cell can then be discretized into a finite number of elements, and solved down the length of the channel. The key assumption to a 1D model is that species transport occurs perpendicular to the channel length dimension.

A variety of assumptions can be made when creating these 1D models. Common assumptions can include isothermal operation, and a constant pressure along the flow channel. The single most commonly referenced model is that of Springer et al[18], which is also one of the earliest models developed. The model is an isothermal 1D model, and is highly focused on predicting the water transport along the length of the flow channel. The transport rate is highly affected by the water saturation of the membrane itself, and much of the emphasis of the work of Springer is related to water transport rate vs membrane humidification levels.

Bernardi et al[19] have produced probably the second most commonly referenced 1D model. This model is also isothermal, and also assumes the membrane is fully
hydrated. Their work, along with the model, greatly stressed the importance of water management in a fuel cell.

A novel idea used by Mazudmer [21] is to solve the most complicated portion of the model, the membrane model, off-line. Then a look-up table can be used to solve a 1D model of the cell [20]. While a great simplification is found using this method, it still does not provide a very simplified control oriented model, nor do models of this level really deal with the properties of pressure drop needed to model the control of system pressure dynamics.

### 2.3.3 2D and 3D Models

The obvious step after a 1D model, is to increase the number of dimension to 2D and 3D models. As the dimension are increased, and assumptions are removed, the
model complexity quickly increases. The models quickly begin to require advanced
CFD techniques to be solved.

These models can involve the complex coupling of linear equations, non-linear
equations, discontinuous equations, partial differential equations, and differential
equations, resulting in the need for complex numerical solution techniques that are
often computationally expensive. [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43].

Models of this level are highly focused on determining properties such as the
local water transfer, local membrane humidity, and local current density. While
these properties are very important to the stack and membrane designers, to a
system integrator, these details are unnecessary. However, for a system integrator
to properly design the anode and cathode supply systems, they will need more
modeling information than just the simple polarization curve.

2.4 Stack Modeling

The modeling reviewed in the previous sections has dealt simply with the mod-
eling of the performance of a single fuel cell. As mentioned in Section 2.1.1, single
cells are typically combined to form a stack to achieve a more usable voltage. When
the cells are combined, the bipolar plates are shared between two adjacent cells. In
this respect, there is much interest in modeling the behavior of the complete stack
from a thermal stand point[43]. To do this, two or more unit cell models can be
combined, and heat transfer from one cell to another can be considered.

Another effect of combining cells is the sharing of the gasses between the inlet
and outlet of the cells. In typical stack construction, there will be some form of
manifold that distributes the anode and cathode gasses to the cells. Typically the gasses enter from one side of the stack, and then are distributed into each individual cell. A study by [40] looks at the effects of flow sharing between cells in a stack, as shown in Fig. 2.8. Its important to model this behavior to see if certain flow designs can be more advantageous, or if unstable designs are possible.

2.5 Pressure Drop Modeling

When considering the design of a fuel cell supply channel, the pressure drop characteristics are an important factor. This is because the supply systems, particularly on the cathode side, are a large auxiliary load on the fuel cells, reducing the overall system efficiency[4, 44]. The most common design recommendations are to keep the flow in the laminar region. Simple laminar flow calculations for incompressible flow in pipes can be used [45, 46]. Equation 2.5 shows a typical example.

$$\Delta P = f \frac{L_{chan}}{D_H} \rho \frac{\dot{v}^2}{2} + \sum K_L \rho \frac{\dot{v}^2}{2}$$  (2.5)

In Eqn. 2.5, $f$ is the friction factor, $L_{chan}$ is the channel length, $D_H$ is the hydraulic diameter, $\rho$ is the fluid density, and $\dot{v}$ is the average velocity, and $K_L$ is
the local resistance. To keep the flow in the laminar region the Reynolds number should be kept below 2300.

This method provides a reasonable and simple approximation of pressure drop for most fuel cells operating on an air supply, but for the BB2 operating on heliox it may not. Wang [47] showed that for a cathode operating on air with an oxygen stoich ratio of 2, the change in density of the gas in the cathode down the length of the channel decreases by only 4%. The BB2, however, is operated on a 40% oxygen mixture, and at a lower stoich ratio. This means that as the cathode reactant travels down the channel, a larger percentage of the cathode gas flow is consumed in the reaction, possibly invalidating the assumptions used to create Eqn. 2.5.

2.6 Modeling with Two Phase Flow

Most of the traditional fundamental fuel cell models are built as single phase models by only considering water in vapor form. The treatment of two phase flow is not particularly simple to deal with, so it makes sense that the earliest models did not attempt to address this problem. However, in any real fuel cell, it is clear the two phases of the water are always present. Numerous groups have, and are still working on understanding this problem[48, 49, 50, 51].

Literature review of two phase flow in fuel cell modeling often results in very detailed models attempting to explain the two-phase properties within the microporous GDL layer [48, 52, 53, 54, 55, 56, 57]. Some of these models even attempt to correlate the phenomena to that of water transport through materials such as dirt, sand and other agglomerates. Models of this type are more focused on predicting
the diffusion properties of the reactants through the GDL to the catalyst, and not interested in looking at the pressure drop along the channel.

Only a few groups have attempted to look at the pressure drop in the channel and taken into consideration two-phase flow characteristics. Rodatz et al. [58, 59] compared the channel pressure drop between single phase and two phase flow calculations, with the two phase flow calculations based on those for direct methanol fuel cells provided by Argyropoulos [52, 53]. Rodatz et al first present a simplified model of single phase pressure drop in a fuel cell, where \( v \) is the mean flow velocity, \( n \) the viscosity, \( l \) the channel length, and \( d \) the hydraulic diameter in Eqn. 2.6.

\[
\Delta p = \frac{v^3 nl}{d^2} \tag{2.6}
\]

Next, they present a simplified model of two-phase pressure drop that was taken from the Argyropoulos model for a direct methanol fuel cell, where \( G \) is the mass velocity, \( y \) the axial co-ordinate, \( v_g \) the specific volume of the gas phase, \( v_{fg} \) the difference in specific volume between the gas and liquid phases, and \( x \) the mass vapor quality.

\[
\Delta p = \int_0^l \left[ G^2(y) \left( \frac{2(yf(y) + K)v_g(y)}{d} \right) \times \left( 1 + \frac{x(y)v_{fg}(y)}{2v_g(y)} \right) \right] dy \tag{2.7}
\]

Large deviations between the model and experimental data were found using the pressure drop Eqn. 2.7. However they did mention that they witnessed a time constant involved in water removal with changes in current draw, as shown in Fig. 2.9 but did not explore the concept any further.

Some recent intriguing work by Wang, Bansu, and Wang [51] does explore the two-phase pressure drop characteristics of flow channels in a fuel cell. They first develop some very complicated 3D equations and use CFD techniques to solve for
some of the two-phase flow properties of the GDL. But later they recognize the importance of the liquid water build up impeding the flow in the channels. They present some very unique concepts. They propose a dimensionless pressure from which they derive a dimensionless pressure drop. From these equations they propose a two-phase pressure factor $\Phi$ shown in Eqn. 2.8.

$$\Phi = \frac{|\Delta P|}{|\Delta P^{1\phi}|} = \int_0^t \frac{1}{1 - s(Y, \zeta, RH_{in})^{n_k}}dY \quad (2.8)$$

In the equation for the two-phase pressure factor, $\Delta P^{1\phi}$ is the theoretical single phase pressure drop, $s$ is liquid water saturation, and $Y$ the dimension along the channel. This means the equation essentially breaks down to a function of $\zeta$, the stoichiometric ratio, and $RH_{in}$, the relative humidity of the inlet gasses. Finally the equation relies on $n_k$, an empirically derived factor that can be used to correct
the two-phase factor to experimental data. This concept is very unique, both in its equation derivation of this two-phase pressure factor, and the use of an empirically tunable parameter to tune the pressure drop to the particular fuel cell.

2.7 System Level Control Modeling

Available models dealing with system level control of fuel cell dynamics are even fewer. Among the most commonly referenced is the model by Pukrushpan et al from the University of Michigan [60, 61, 62, 63]. This model relies on a constant temperature assumption, and uses lumped volumes and ideal gas equations to form the basis of the cathode and anode dynamics. The control volumes are essentially divided into inlet and exhaust volumes. The mass balance due to the fuel cell reaction is considered to occur in the inlet control volume. Then a linearized stack resistance is used to determine pressure drop across the stack to the exhaust volume. Then another linearized resistance is used to calculate the back pressure on the stack. Much more detail on this model will be provided in Chapter 3.

Several fundamental problems are found with the assumptions, and model linearizations used in [60]. One assumption of the model is that the liquid water that forms in the cathode is essentially ignored. The mass of the liquid water is accounted for, but it is assumed to not affect the pressure drop characteristics of the cell, assumed not to exit the inlet volume, and assumed to not obstruct the flow of reactants through the gas channel. In an actual fuel cell system, none of these assumptions are true. The liquid water drastically effects the pressure drop because it obstructs the flow of reactants, and a significant amount of the liquid water exits the stack. These assumptions may be more valid on lower powered fuel cell systems
operating on air, but they do not work well for the high power BB2 fuel cell system running with heliox.

Another simplification of the model is the linear stack resistance that is assumed proportional to mass flow rate, and taken into account after the fuel cell reaction. In reality there is a complex interaction along the length of the channel as oxygen is consumed, and turned into water.

Another lumped parameter system level model is created by Xue et al\cite{64}. This group differs from the model of \cite{60}, by considering the temperature and thermal effects for three separate control volumes, the anode, cathode, and the MEA. The group considers the combined effects of temperature, gas flow, and capacitance, specifically for the purposes of analyzing transient behavior. Unfortunately they still do not consider the effects of liquid water in their model, and still use simplified upstream and downstream linearized resistances.

### 2.8 Conclusion

This chapter has provided a required background in fuel cells and the current status of their modeling. The basic operation of fuel cells was first detailed. Next some comments on the application of fuel cells to automotive transportation were given, showing the current status of the technology. A background on 1D and 3D modeling of single cells was also covered. Finally it was shown that comparatively little work has been done on the modeling of the complete system, especially with regards to the pressure dynamics involved when dealing with liquid product water.
CHAPTER 3

Modeling of the BB2 System

This chapter provides the details of the models that have been developed for the BB2 system. The chapter begins by providing a basic overview each of the fuel cell supply systems. Detailed descriptions of the anode, cathode, and cooling system are provided.

Next, the chapter provides the detailed equations used in the adaptation of the model of [60] to the BB2 system. In order to adapt this model, a new exhaust system and back pressure valve model are developed. Next a simple modification to this model is proposed to account for the effects of water exiting the cathode model.

Finally, a laminar flow model is proposed as a method for predicting the water outlet flow rate. First, the simplified equations used to calculate laminar flow are provided. Next, a discretized model is developed that involves the solution of a laminar flow model with gas and water flowing separately through a fuel cell channel. The details of the solution are provided. The discretized laminar flow model is then presented with both a single upstream stack resistance, and a split upstream and downstream resistance.
3.1 Layout and System Description

The BB2 fuel cell system layout is shown in Fig. 3.1. The system consists of two Fuel Cell Modules (FCMs) operated in parallel. Each FCM must be supplied with hydrogen at the anode, oxygen at the cathode, and a liquid coolant. The details of each of these systems will be given in the following sections.

3.1.1 Anode System

Hydrogen is supplied from a single storage tank to each FCM, and each FCM controls the pressure and recirculation of the hydrogen gas. In a fuel cell, electrons are stripped from hydrogen molecules and conducted through an electrical circuit.
Theoretically, hydrogen only needs to be supplied to the fuel cell at the rate it is consumed. This is impractical because as hydrogen flows through the stack and is consumed, the hydrogen concentrations will reach zero at the outlet. In reality, the partial pressure and the concentration needs to be much higher for the reaction to be efficient. Hydrogen gas must be supplied at a higher mass flow rate than it is consumed. The unreacted gas exiting the stack is recirculated back to the inlet via a jet pump. During normal operation, water and other contaminants may migrate from the cathode across the membrane and accumulate in the fuel loop. The fuel loop must be periodically purged to clear out these contaminants. The wasted hydrogen is accounted for in a hydrogen utilization factor $\mu$. Typically, only a small percentage of the total fuel is wasted to satisfy purge cycle requirements.
The rate of hydrogen consumption is proportional to the current drawn from the stack. The mass flow rate of hydrogen can be calculated for a given current. In Eqn. 3.1 the current is divided by Faraday’s constant (the amount of charge in 1 mole of electrons), the number of electrons per molecule of hydrogen, and multiplied by molar mass of hydrogen and the number of cells in series.

\[
\dot{m}_{H_2} = \frac{I}{2F} M_{H_2} \frac{1}{\mu} N_{cells}
\]

(3.1)

### 3.1.2 Cathode System

The cathode supply system for the two FCMs is operated in parallel with a shared exhaust and pressure regulation system. To maximize fuel cell performance, the cathode system uses “heliox”, a mixture that contains 40% oxygen and 60% helium. Under high current operation, fuel cells suffer from losses referred to as concentration losses. These are the result of low concentrations of the reactant gases near the reaction site on the membrane. The enriched oxygen content provided by the heliox increases the oxygen concentration, and reduces voltage losses at high current draws.

The heliox is stored in two bulk storage tanks, near a maximum of 220 bar. The tank pressure is regulated to 10 bar, just upstream of two mass flow controllers. The mass flow controllers regulate the flow rate to each FCM independently. The cathode gases flow into each FCM, where they pass through a Ballard-designed humidifier before entering the fuel cell stack.

After the cathode gases pass through the fuel cell stack the gases are combined in a shared exhaust volume. While the flow rate of the heliox is controlled by the mass flow controllers, the heliox operating pressure is controlled by three internally
piloted pressure regulation valves. These valves allow gases to exit from the shared exhaust volume while simultaneously regulating the back pressure of the cathode system.

Similar to the anode, the cathode gases must also be supplied at a flow rate higher than their actual consumption. Specifically the oxygen must be supplied at a higher rate than the oxygen is consumed. The measurement of this excess flow is called the oxygen excess ratio, or more commonly the oxygen stoichiometric (stoich) ratio. This is the ratio of the supplied oxygen to the consumed oxygen.

\[ \lambda_{O_2} = \frac{W_{O_2,\text{in}}}{W_{O_2,\text{reacted}}} \]  

(3.2)

The rate of the oxidant supply can then be determined based on the desired stoich ratio and the oxygen content of the supply gas, \( ppO_2 \).

\[ \dot{m}_{O_2} = \frac{I}{4F} \frac{M_{O_2}}{ppO_2} \lambda N_{\text{cells}} \]  

(3.3)

For a normal fuel cell vehicle, since the oxygen is typically drawn from the air, supplying extra air does not directly result in excess fuel consumption, although there will be an overall system penalty due to the parasitic loss from running the compressor if the stoich ratio is set far too high. The typical ratio that results in acceptable performance with minimal parasitic loss for air is a stoich ratio around 2.

The flow of the cathode gases serves two purposes. One is to supply the oxygen for the fuel cell reaction. The second purpose is to aid in the removal of product water. When air is used, with an oxygen concentration of approximately 21% Oxygen, and 79% Nitrogen, an oxygen stoich ratio of 2 brings along a lot of nitrogen to help remove the water. In the case of the BB2, running 40% Oxygen, and 60%
Helium, not as much extra gas will be available to remove the product water at an equivalent stoich ratio. In addition, since the gases for the BB2 are stored in a limited supply, the stoich ratio was actually reduced slightly to allow the vehicle to complete it is entire run without depleting the supply tank. This ultimately means that water removal is not as well facilitated in the BB2 as it would be in a normal fuel cell vehicle.

3.1.3 Cooling System

One of the challenges for a fuel cell system is the removal of heat. A PEM fuel cell stack could theoretically operate above 70% efficiency, but the efficiency decreases with increasing current density [4]. The Buckeye Bullet 2 is pushing the current density to nearly the peak power point of the fuel cells, which is a region that operates at approximately 50% efficiency. That means that if there is 500kW of electrical power produced, an equal amount of thermal energy must be removed. The use of a traditional liquid-air radiator was quickly eliminated due to the aerodynamic drag imposed by the large cooling requirements of the fuel cells.

The cooling system for the BB2 is a two loop system, with a heat exchanger removing heat from the primary loop to the secondary loop through a liquid to liquid heat exchanger. The primary loop goes through the fuel cells, a pump, and the heat exchanger. It contains deionized water, since it runs through the fuel cells and is in contact with high voltage. The secondary loop contains regular water, and goes through an ice bath, pump, and the heat exchanger.

Ideally, the fuel cells would be held at an operating temperature of 80 °C, with an inlet temperature of 65 °C, so the $\Delta T$ across the stack is maintained at 15 °C.
Figure 3.3: Cooling System Block Diagram.

Luckily the desired thermal cycle is very predictable. To maintain this temperature differential, the flow rate of the secondary loop is regulated with a feedback controller. Details of the design and control of the cooling system are provided in the work of Ponziani[65].

3.2 Control Level Model Development

This section details the development of the BB2 fuel cell system model that is based off the work of [60]. The model used in [60] separates the fuel cell system into two separate control volumes, the cathode volume, and the exhaust volume. Into the cathode volume flow the inlet gases. Within this control volume the gases are reacted or generated due to the fuel cell reaction, and gases may leave through the stack resistance. gases may then enter the exhaust control volume, and exit through an exhaust resistance.
In the BB2, two FCMs are routed in parallel with their exhaust gases flowing into a shared exhaust volume. This model has to make two changes to deal with the physical layout to the BB2 fuel cell system. Two separate cathode volumes must be considered separately, and their outlets must be combined in an exhaust manifold that accounts for the potentially different mixture of gases entering the exhaust manifold. The complete cathode and exhaust system model layout is shown in Fig. 3.5.

The development of the cathode model will be detailed in the next section, followed by the details of the exhaust volume.

### 3.2.1 Cathode Model

The details of both fuel cell module cathode subsystems are identical, there is simply one version used for Module A, and one for Module B. Each module receives different airflow and current inputs that are obtained from the test data. The final
input to the cathode model is the exhaust manifold pressure which is fed back from the exhaust manifold model.

The Cathode Subsystem model is shown in Fig. 3.6. The model consists of 6 separate blocks: Inlet Flow and Humidifier, Cathode Mass Balance, Electro Chemistry, Cathode Mass Balance, Thermodynamic Calculations, Stack Resistance, and Outlet Flow Properties. A description of the major blocks of the model is given below, along with their basic equations. Full details of the equations can be found in [60].
Figure 3.6: Block Diagram of the cathode subsystem of the control oriented model for the BB2.

**Inlet Flow and Humidifier**

The Inlet-Flow-and-Humidifier-Block takes the flow rate that is recorded by the mass flow controller, and calculates the amount of water that must be injected to create a saturated flow stream. The input to the block is simply the mass flow rate of heliox that is recorded by the mass flow controller, as well as the system operating temperature, and the pressure which is fed back from the thermodynamic calculations block. Equation 3.4 can then be used to calculate the mass of water
that must be injected to the stream to reach the desired saturation condition.

\[
W_{v, \text{inj}} = \frac{M_v}{M_{\text{heliox}}} \frac{\phi_{\text{des}} P_{\text{sat}}(T)}{P_{\text{ca}}} W_{\text{heliox, mfc}}
\] (3.4)

In the case of the modeling used for the BB2, due to the robust design of the Ballard humidification system, and its integrated water trap, the assumed desired relative humidity will always be set at 100%. The Inlet Flow and Humidifier block finishes by separating the flow into the individual mass flow rates of oxygen, helium, and water vapor that enter the cathode volume. A slight difference in the model when applied to the BB2 vs. that in [60] is that the cathode gas is heliox. Because of this the inlet gases to the cathode mass balance block are simply oxygen, helium, and water vapor, instead of oxygen, nitrogen, and water vapor.

**Cathode Mass Balance Block**

The Cathode-Mass-Balance-Block tracks the mass of each component of the cathode volume. Oxygen, helium, and vapor enter the volume. Based on the fuel cell reaction, oxygen can be consumed, and replaced with water vapor. Oxygen, helium, and vapor may leave the cathode volume based on the calculations from the outlet flows block. The equations for the reacted and generated term are detailed below in the section on the electro chemistry block. The following equations show how the inlet, outlet, and reacted/generated mass flow rates are used to calculate the mass of the individual species.

\[
\frac{dm_{O_2,\text{ca}}}{dt} = W_{O_2,\text{ca,in}} - W_{O_2,\text{ca,out}} - W_{O_2,\text{reacted}}
\] (3.5)

\[
\frac{dm_{\text{He,ca}}}{dt} = W_{\text{He,in}} - W_{\text{He,out}}
\] (3.6)

\[
\frac{dm_{v,\text{ca}}}{dt} = W_{v,\text{ca,in}} - W_{v,\text{ca,out}} + W_{v,\text{gen}} - W_{l,\text{ca,out}}
\] (3.7)
The creation of liquid water is also calculated and tracked in the cathode volume. This is done by calculating the saturation pressure of water vapor, based on the fuel cell temperature. Using the volume of the cathode, the maximum mass of water vapor that can be held in the cathode can be calculated. If more water is present in the cathode than the saturation conditions allow, then liquid water is formed. The equation used for saturation pressure is shown in Eqn. 3.8, with \( p_{\text{sat}} \) in kPa.

The maximum mass of vapor allowable is shown in Eqn. 3.9.

\[
\log_{10}(P_{\text{sat}}) = -1.69e^{-10}T^4 + 3.85e^{-7}T^3 - 3.39e^{-4}T^2 + 0.143T - 20.92 \tag{3.8}
\]

\[
m_{v,\text{max,ca}} = \frac{p_{\text{sat}}V_{ca}}{R_gT_{st}} \tag{3.9}
\]

Knowing the maximum mass of vapor the system can hold, and the water mass from the mass balance equation, the amount of liquid water can be calculated as follows.

If \( m_{w,ca} \leq m_{v,\text{max,ca}} \rightarrow m_{v,ca} = m_{w,ca}, m_{l,ca} = 0 \) \hspace{1cm} (3.10)

If \( m_{w,ca} > m_{v,\text{max,ca}} \rightarrow m_{v,ca} = m_{v,\text{max,ca}}, m_{l,ca} = m_{w,ca} - m_{v,\text{max,ca}} \) \hspace{1cm} (3.11)

According to the assumptions used in [60], liquid water is ignored if it is generated. The liquid water does not affect the pressure of the cathode, and is assumed to not leave the cathode. This will later be shown to be a major downside of the model. The mass of liquid water accumulated in the cathode volume is tracked by this model, and turns out to be quite significant under the operating conditions of the BB2.

**Thermodynamic Calculations Block**

The Thermodynamic-Calculations-Block is where the pressure is calculated using Dalton’s law. With a fixed cathode volume, and the known mass of gas from the
mass balance block, the pressure of the cathode volume is calculated using a constant temperature assumption. In [60], the fuel cell temperature is assumed constant, at a fixed temperature. This model only slightly deviates from that assumption, and uses the recorded temperature from test data as an input when simulations are run. The generic equation used for each component is given in Eq. 3.12. A separate equation is used for each component, where the term \( i \) is replaced with \( O_2 \) for the oxygen mass balance, \( He \) for the helium mass balance, and \( v \) for the vapor mass balance.

\[
p_i = \frac{m_{i,ca} R_i T_{st}}{V_{ca}} \tag{3.12}
\]

Because the tracking of liquid water is not considered, the cathode volume is considered constant in the work of [60], and the same assumption is used in the initial model development here.

**Stack Resistance Block**

The Stack-Resistance-Block uses a linearized stack resistance to calculate the flow out of the cathode. The outlet mass flow rate is calculated based on the difference between the cathode pressure, and the exhaust manifold pressure, which is calculated in a separate model for the exhaust manifold volume. The linearized equation for the mass flow rate through the cathode is shown in Eq. 3.13.

\[
W_{ca,out} = K_{stack}(P_{ca} - P_{em}) \tag{3.13}
\]

The assumption of the linear stack resistance is one that requires some discussion. There are two reasons this assumption can be somewhat valid for the BB2. The first is that the BB2 operating conditions are mainly at a constant full throttle flow rate for most of the area of modeling concern. If a vehicle were to operate
in a wider range of conditions, perhaps this assumption should be re-investigated. Another reason to consider this is that the channels of the stack operate under laminar flow conditions, with a relatively small pressure ratio. Under these types of flow conditions, it is quite common to formulate a flow rate that is proportional to the pressure difference.

**Outlet Flow Properties Block**

The Outlet-Flow-Properties-Block calculation uses the mass mixture of the gas in the cathode to convert the outlet mass flow rate into the mass flow rates of the individual components. The inputs to the block are the outlet flow rate, and the component masses within the cathode. Knowing the masses of the component gases, the mass fraction of each gas can be calculated based on the total mass of all the gases.

\[ m_{\text{total}} = m_{\text{O}_2,\text{ca}} + m_{\text{He,ca}} + m_{\text{H}_2\text{O},\text{ca}} \]  
(3.14)

\[ X_i = \frac{m_i}{m_{\text{total}}} \]  
(3.15)

Finally it is possible to calculate the cathode outlet flow rates for each individual species based off the outlet flow rate and the mass fraction, as shown in Eq. 3.16.

\[ W_{i,\text{ca, out}} = X_i W_{\text{ca, out}} \]  
(3.16)

**Electrochemistry Block**

The Electrochemistry-Block calculates the consumption of the oxygen proportional to the current draw. The recorded current draw is an input to this block. The oxygen is replaced with water vapor according to the chemical reaction for the formation of water. The equations for the consumption of oxygen and generation of
water are shown below.

\[ W_{O_2, reacted} = M_{O_2} \times \frac{n_{st}}{4F} \]  
\[ W_{V, generated} = M_v \times \frac{n_{st}}{2F} \]  

(3.17)  
(3.18)

Membrane Water Transfer

Discussion of the membrane water transfer model used in [60] is required. Water can be transported across the membrane through a few separate mechanisms. First it can be dragged across the membrane toward the cathode as the protons move from the anode the cathode, this process is called electro-osmotic drag. The second mechanism is from diffusion that can naturally occur when the concentration of water is less on one side of the membrane. This typically occurs from the cathode to anode. These two mechanisms are highly dependent on the water content of the membrane itself. A third mechanism can be due to any pressure gradient that might exist between the anode and cathode. In the case of the BB2 the anode always has positive pressure with respect to the cathode.

These phenomena are very complex. The membrane model used in [60] showed poor results. During simulations the membrane model in [60] always resulted in membrane dehydration. Because of the poor performance of this portion of the model, it was not used in the presentation of the results in [60].

The BB2 runs at extremely high current densities, and produces massive amounts of product water. Testing results show that the amount of water that is removed from the anode water trap during a run are fairly insignificant compared to the massive liquid and water vapor streams that pour out of the cathode during high current operation.
The modeling done in this dissertation will ignore membrane water transfer, and assume all product water is formed on the Cathode side due to the reasons discussed above.

### 3.2.2 Exhaust Manifold Equations

A further modification from the model in [60] comes from the treatment of the exhaust manifold. The model in [60] uses a single fuel cell stack, and a single exhaust manifold volume. However the BB2 runs two stacks in parallel, with a shared exhaust manifold volume. This means it is possible that the composition of gases entering the exhaust manifold from Module A and B could be different, and the mixture of gases in the exhaust manifold needs to be calculated. To handle this modeling problem, the exhaust manifold is set up with a similar structure to the cathode volume, and a block diagram of the exhaust volume for the BB2 model can be seen in Fig. 3.7.

**Exhaust Manifold Mass Balance Block**

A Mass-Balance-Block similar to the cathode volume is used to track the mass of each component in the exhaust manifold. Oxygen, Helium, and Water Vapor can enter the volume from FCMA and FCMB. The mass balance equations are rewritten as follows.

\[
\frac{dm_{O_2,em}}{dt} = W_{O_2,ca,A,out} + W_{O_2,ca,B,out} - W_{O_2,em,out} \quad (3.19)
\]

\[
\frac{dm_{He,em}}{dt} = W_{He,ca,A,out} + W_{He,ca,B,out} - W_{He,em,out} \quad (3.20)
\]

\[
\frac{dm_{w,em}}{dt} = W_{w,ca,A,out} + W_{w,ca,B,out} - W_{w,em,out} \quad (3.21)
\]
Figure 3.7: Block Diagram of the Exhaust Manifold Model.

There are two major deviations between Eqs. 3.5-3.7 and Eqs. 3.19-3.21. The first is that there are two inlet terms from each fuel cell module. The second difference is that there are no generation or reaction terms from the fuel cell reaction electrochemistry, because no reactions occur in the exhaust manifold.

Liquid water formation is tracked exactly as it is in the cathode volume, except the exhaust manifold volume is used to calculate $m_{v,max}^\text{em}$.

\[
m_{v,max}^\text{em} = \frac{p_{\text{sat}}V_{em}}{R_vT_{st}}
\]  

(3.22)
If \( m_{w,em} \leq m_{v,max,em} \rightarrow m_{v,em} = m_{w,em}, \ m_{t,em} = 0 \) \hspace{1cm} (3.23)

If \( m_{w,em} > m_{v,max,em} \rightarrow m_{v,em} = m_{v,max,em}, \ m_{t,em} = m_{w,em} - m_{v,max,em} \) \hspace{1cm} (3.24)

The mixture of gases in the volume is allowed to exit at a flow rate determined by the back pressure valve model, which will be discussed below in Section 3.3.

**Exhaust Manifold Thermodynamic Calculations**

The Thermodynamic-Calculations-Block operates exactly as it does in the cathode volume, using Dalton’s law and the mass of the individual gases in the volume to calculate the instantaneous pressure of the exhaust manifold. The generic equation for any species gas, \( i \), is given below. The total system pressure is then the summation of the partial pressures of the three gases in the exhaust manifold.

\[
p_{i,em} = \frac{m_{i,em}R_{i}T_{st}}{V_{em}}
\]

\[
p_{em} = p_{O_{2},em} + p_{He,em} + p_{v,em}
\]

A new calculation used within the thermodynamic calculations block is the calculation of the specific gravity of the gases. This is needed for the back pressure valve model and its equation is provided below. The specific gravity is the density of the gas in the exhaust manifold relative to the density of air.

First the two densities must be calculated. The exhaust manifold gas density can simply be calculated because the mass of the gases is known from the mass balance block. The total mass in the exhaust manifold is given in Eq. 3.27. Dividing the total mass by the volume of the exhaust manifold provides the density of the gases in the exhaust manifold.

\[
m_{total,em} = m_{O_{2},em} + m_{He,em} + m_{v,em}
\]

50
\[ \rho_{em} = \frac{m_{total,em}}{V_{em}} \]  

(3.28)

The only remaining item needed to calculate the specific gravity is the density of air at the same pressure and temperature. This is calculated from the ideal gas law. Then the specific gravity of the exhaust gas can be calculated.

\[ \rho_{air,em} = \frac{P_{em}}{R_{air}T_{em}} \]  

(3.29)

\[ SG_{em} = \frac{\rho_{em}}{\rho_{air}} \]  

(3.30)

The specific gravity of the exhaust gas, along with the exhaust manifold pressure, and mass fractions of the gases in the exhaust manifold are all sent to the back pressure valve model, which calculates the outlet flow rates from the exhaust manifold. Similar to the outlet flow properties block used in the cathode model, the outlet flow rate of the individual gas components is calculated proportionally to the mass fraction of the gases in the exhaust manifold. Then the outlet flow rate is multiplied by the number of back pressure valves that are operating in parallel.

3.3 Back Pressure Valve Model Development

The term back pressure is used to refer to the pressure downstream of the fuel cell stack, and in this model it is equivalent to the pressure seen in the exhaust manifold. In a conventional fuel cell system, under steady state conditions, the pressure drop across the stack is fairly consistent. Therefore controlling the back pressure is normally an acceptable method to control the stack operating pressure.

To simplify the tuning and control of the BB2 system, a passive back pressure control device was used, and is referred to as the back pressure valve (BPV). For the BB2 a Fischer 289H 1inch BPV was selected, and it is shown in Fig. 3.8. To meet
flow rate and packaging requirements, 3 BPV’s are used in parallel. The valve is internally piloted, and adjustable to various pressure settings through an externally adjustable screw that preloads a spring against a diaphragm. The internally piloted pitot tube can create a vacuum on the back side of the diaphragm to open the valve further with increasing flow rate, leading to relatively flat pressure operation over a wide range of flow rates.

Figure 3.8: Fischer 289 valve used in the BB2 as a back pressure valve.

To create a model of the BPV, the manufacturer’s data sheet is used, which is shown in Fig. 3.9. The data sheet provides a volumetric flow rate based the inlet pressure, and the valve’s adjustable pressure setting.
Figure 3.9: Fischer Valve Performance provided by the manufacturer for 0.6 SG dry gas.

The manufacturer’s flow map provides lines for a variety of pre-set pressure settings. Because the final setting of the BPV will not fall on a single line, the lines are turned into an exponential curve fit from the data read off the flow chart. These curve fits are used to create a flow map. In addition, the map is inverted, because the input to the model will be the inlet pressure, and the output will be volumetric flow rate of the gases. This map is shown in Fig. 3.10.

The flow map is based on a 0.6 SG gas, but correction factors are provided for a variety of standard industrial gases based on their SG. Because the SG of the
exhaust gases will be changing instantaneously with the composition of the exhaust manifold, a curve fit for the SG to the correction factor is created. This curve fit uses the SG of the exhaust manifold, and calculates the instantaneous correction factor for the flow map. This curve fit is shown in Fig. 3.11.

The complete model for the back pressure valve uses the exhaust manifold pressure, and the exhaust manifold specific gravity to calculate the exiting flow rate from the exhaust manifold.

### 3.3.1 Pressure Relief Valve Model

As an additional safety feature, pressure relief valves were installed between the humidifier and the cathode inlet. The pressure relief valves are set to be inactive during normal operation. During transient conditions, or in the case of a full-open
failure of the mass flow controller, the pressure relief valves open to vent excess pressure. The pressure relief valves were active during the race events for the BB2. Chapter 4 provides many details on the testing and tuning of the pressure relief valves. For model validation testing conducted statically for a part of this research, the valves were set to be inactive by significantly increasing their pressure setting.

3.4 Cathode Model with Simplified Two Phase Flow Considerations

One of the key features that is not accounted for in the previous model is that the pressure drop model does not account for the gas and liquid water that are flowing together through the flow channels. The difference in pressure between the cathode and the exhaust manifold defines the flow rate. However the model in [60] assumes this pressure difference drives only the gas portion of the flow, and the linearized
flow Eqn. 3.13 relates the pressure drop to a mass flow rate of gas only. In reality, understanding and modeling the complex interaction of tiny water droplet along tiny flow channels is very complex [67].

As a first approximation, it is possible to adopt a phenomenological representation of the phenomena described above by assuming that the water exit flow rate is proportional to the mass of the water within the cathode. This allows for modifying Eqn. 3.13 as follows:

\[ W_{ca,\text{out}} = K_{\text{stack}}(P_{ca} - P_{em}) \] (3.31)

Although Eqn. 3.13 appears identical to Eqn. 3.31, the term \( W_{ca,\text{out}} \) in 3.31 will be allowed to include both a mass flow of water and a mass flow of gas. Many papers have shown experimental visualization of water build up in cathode channels [67, 50]. It is well known that water may build up along the wall, and not all of it will necessarily flow out at the rate it is generated.

The key assumption for this model modification is that the mixing of the water droplets into the gas flow stream is assumed to be proportional to the mass of water that is accumulated in the cathode. As more water builds in the cathode, the gas channels will become more restricted, and push more liquid water droplets out of the cathode.

The previously developed model in this paper tracks the instantaneous mass of liquid water that is formed in the cathode. The mass fractions, \( X \), of the gases and liquid are calculated as follows.

\[ X_g = \frac{m_{ca} - m_L}{m_{ca,\text{total}}} \] (3.32)

\[ X_L = \frac{m_L}{m_{ca,\text{total}}} \] (3.33)
If the flow was a perfect mixture of the gas and liquid proportional to its mass fractions, the mass flow rate of the gas and liquid could be calculated as follows, with the subscript tp indicating perfectly mixed two phase flow.

\[ W_{g,ca,out,tp} = W_{ca,out} \times X_g \]  
\[ W_{L,ca,out,tp} = W_{ca,out} \times X_L \]  

The liquid flow, however, will only be a portion of this perfectly mixed flow, and will be dependent on the amount of water that has accumulated in the channels. A calibration parameter is introduced to help drive this proportionality, and is the maximum mass of liquid water that can be held in the fuel cell stack \( m_{L,ca,max} \).

The proportion of liquid mass flow can be determined with the following equation.

\[ K_L = \frac{m_{L,ca}}{m_{L,ca,max}} \]  
\[ W_{L,ca,out} = W_{L,ca,out,tp} \times K_L \]  

Once the liquid outlet flow rate is known, the mass flow rate that is not used by the liquid is added to the gas mass flow rate that is allowed to exit, as follows.

\[ W_{g,ca,out} = W_{g,ca,out,tp} + (W_{L,ca,out,tp} - W_{L,ca,out}) \]  

Although the proposed approach is extremely simplified, it provides a quick method to evaluate the effects of the water generation on the flow resistance through the cathode, providing guidelines for more thorough model development.

### 3.5 Two-Phase Exhaust and Back Pressure Valve Model

The previously detailed model of the exhaust manifold tracked the formation of liquid water, but similar to the work of [60], the liquid water formation was ignored.
The exhaust manifold and back pressure valve models need to be modified to handle the liquid water.

### 3.5.1 The two-phase exhaust manifold model

While a detailed model will be developed to allow different flow rates for the gas and liquid phases in the cathode, that type of model is not very applicable to the exhaust manifold. The flow through the exhaust manifold is the result of all the exiting gases flowing through large silicone tubes and aluminum piping. The cathode has the gas diffusion layer, and very small channels under laminar flow conditions, so it is very capable of having a liquid water separated from the gas flow. The flow conditions in the exhaust tubing are quite different, under turbulent flow conditions, and there are not really any good mechanisms to trap and hold the liquid water. Because of this difference, it is fairly reasonable to assume that the liquid water droplets are evenly dispersed in the flow proportional to their mass fraction, and a much simpler model can be developed.

The exhaust manifold model is modified to handle the two phases by considering that the liquid water will exit proportionally to its mass fraction in the exhaust manifold. Thus if a certain exiting gas mass flow rate is determined from the back pressure valve model, the water will exit proportionally to its two phase mass fraction in the exhaust volume. To understand this new two phase consideration, two phase liquid mass fraction is shown in the equations below.

\[
m_{total,em,tp} = m_{O_2,em} + m_{He,em} + m_{v,em} + m_{L,em}
\]

\[
X_{L,em,tp} = \frac{m_{L,em}}{m_{total,em,tp}}
\]

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The total exiting mass flow rate is a combination of the liquid and gas flows. The exiting gas flow rate $W_{g,em,out}$ will be determined from the new two phase back pressure valve model detailed below in Section 3.5.2.

$$W_{em,out,total} = W_{g,em,out} + W_{L,em,out} \quad (3.41)$$

The liquid exiting flow rate is equal to the total rate times the two phase liquid mass fraction.

$$W_{L,em,out} = W_{em,out,total} X_{L,em,tp} \quad (3.42)$$

To determine the liquid exit flow rate as a function of the gas exit flow rate, Eqns. 3.41 and 3.42 can be combined, and solved for the liquid exiting flow rate.

$$W_{L,em,out} = W_{g,em,out} \left[ \frac{X_{L,em,tp}}{1 - X_{L,em,tp}} \right] \quad (3.43)$$

The mass Balance Eqn. 3.21 is rewritten to include the liquid water that is calculated to exit the exhaust volume.

$$\frac{dm_{w,em}}{dt} = W_{v,ca,A, out} + W_{v,ca,B, out} - W_{v,em, out} - W_{L,em,out} \quad (3.44)$$

It is worthwhile to mention that to fully consider liquid water in the exhaust manifold, the volume available for the gases would effectively be reduced. However, for the large exhaust volume, the data analysis shows the actual mass of the water in the exhaust manifold is very small, and its volume negligible compared to the total volume of the exhaust manifold.

### 3.5.2 The Two Phase Back Pressure Valve Model

The treatment of two phase flow through the back pressure valve is not an easy modification to make. When dealing with dry gas flows, it is fairly easy to use
the data sheet from the manufacturer, and the suggested correction factor based on the SG of the gas to determine the new flow rate when the valve setting and inlet pressure are known. To consider the effect of the water droplets entrained in the gas mixture requires a reexamination of the back pressure valve model to account for the water.

For the treatment of two phase flow, the data sheet from the manufacturer will be used to create a more physical representation of how the back pressure valve is operating. The data sheet was shown in Fig. 3.9, and gives flow rate vs. inlet pressure for a variety of preset valve settings. Each line represents a pressure setting, and it is possible to tune the valve to operate in between any of the lines on the sheet, but it will follow the trend defined by the lines. The data in Fig. 3.9 is provided for natural gas, the typical gas the valve was designed for.

Figure 3.12 show the steps used in the calculations for the new model that will deal with two phase flow. Figure 3.12(a) shows the data from the manufactures sheet in dashed colored lines. Each line represents one of the preset lines corresponding to a setting in psi. For example the green line corresponds to the 40 psi setting. The data in Fig. 3.12(a) is presented in English units with a gauge pressure setting as the input pressure, using the same units used in Fig. 3.9.

The solid lines in Fig. 3.12(a) represent the lines that are used for model development, and are a modification from the provided data sheet. This is required due to the small knee in the data sheet at low flow rates. The valve has a cracking pressure that leads to a small pressure rise, and once its cracked the valve’s internal pitot tube will open the valve further and reduce the upstream pressure slightly. Unfortunately, this leads to behavior that would be difficult to model, because there
could be multiple flow rates for a given input pressure. The final model will have pressure as the input and flow rate as the output, so there needs to be a one to one relationship for pressure to flow. For this reason the lines are smoothed out so the flow can be calculated directly from the pressure. This is a negligible modification, and quite insignificant because in the BB2 the valve will operate in much higher flow conditions.

Figure 3.12(b) simply shows the same data, but converted to SI units of flow rate in \( m^3/s \) and inlet pressure in absolute bar. Figure 3.12(c) shows the same data, but the volumetric flow rate on the x-axis has been converted to a mass flow rate based on the atmospheric temperature and pressure provided on the data sheet.

Next, Fig. 3.12(d) shows the same mass flow rate lines, and how the data lines can be interpolated to get a new pressure vs flow line based on a new valve setting. The example shown in Fig. 3.12(d) is for a 35 psi setting.

From these flow vs. pressure lines, the effective \( C_dA \) of the valve is calculated assuming choked flow conditions. The equations for this calculation are based on the equations for fluid flow through a restriction found in [68]. The equations in [68] are derived for two conditions, normal flow, and choked flow conditions. To check for choked flow conditions, the critical pressure ratio must first be calculated. Sample calculations are provided below for natural gas, the working fluid from the back pressure valve data sheet. The following equation is used to calculate the critical pressure ratio, where \( P_1 \) is the upstream pressure and \( P_2 \) is the downstream pressure, and \( \gamma \) is the ratio of specific heats. Sample numbers are used for natural gas as the working fluid, with \( \gamma = 1.27 \).
\[
\frac{P_2}{P_1} = \left( \frac{2}{\gamma + 1} \right)^{\gamma - 1} = \left( \frac{2}{1.27 + 1} \right)^{\frac{1.27}{1.27 - 1}} = 0.55
\] (3.45)

If the pressure ratio is below the value in Eqn. 3.45, then the restriction is operating in choked flow conditions. For the BB2 a typical back pressure is about 2.2 bar-gauge, or about 3.2 bar-absolute. The outlet pressure is always atmospheric, about 1.0 bar-absolute, so the pressure ratio is typically on the order of 0.31 which is well below the critical pressure ratio of 0.55. Even accounting for slight changes in the value of \(\gamma\), its very unlikely the pressure ratio would ever be near that of non-choked conditions.

Since it is shown that in all cases the flow will be that of choked flow, the inlet pressure and flow rate can be used to calculate the effective area, \(C_dA\). Equation 3.46 gives the mass flow rate through an orifice under choked flow conditions, where \(P_1\) is the upstream pressure, \(C_d\) is the flow coefficient, \(A_T\) is the throat area, \(R\) is the gas constant for the working gas, \(T\) is the temperature, and \(\gamma\) is ratio of specific heats [68].

\[
W_{\text{Choked}} = \frac{C_d A_T P_1}{\sqrt{RT}} \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma + 1}{\gamma(\gamma - 1)}}
\] (3.46)

The above equation can be solved to give the effective area, \(C_dA\) for any combination of mass flow rate and inlet pressure. The results of this calculation are shown in Fig. 3.12(e) for each of the preset flow conditions, with a sample line representing the \(C_dA\) vs inlet pressure interpolated for a 35 psi valve setting.

With the valve’s \(C_dA\) known for a given inlet pressure and valve pressure setting, the outlet flow rate of any new gas composition can then be calculated using Eqn. 3.46 by using the value for \(R\) and \(T\) of the upstream gases. Figure 3.12(f) shows
some sample curves of gases with various specific gravities. An SG of 1.00 would be for air, and Sg of 0.55 would be for unreacted heliox, and an SG of 0.35 represents a typical value of the gases during full current draw after they have passed through the cathode.

To this point, the back pressure valve model has simply been recalculated using a different method to account for the varying specific gravity of the gases. To account for the two phase flow, the last calculation of the mass flow rate, which depends on the calculated \( C_d A \) will be affected by changing the \( C_d A \). With water droplets entrained in the flow, they will essentially be reducing the effective area of the valve, and its flow properties represented by simply \( C_d \).

Intensive bench testing could be used to fully characterize this valve under a variety of two-phase flow conditions, but this was impractical to conduct. Instead, a simple tunable coefficient, \( K_{BPVT} \), needs to be introduced. The coefficient will be used to reduce the effective \( C_d A \) based on the quantity of water in the exhaust manifold according to the equation below.

\[
C_d A_{tp} = C_d A - K_{BPVT} m_{L,em} \tag{3.47}
\]

This coefficient can be tuned until the model reflects the pressure rise that occurs as more and more liquid is introduced into the exhaust outlet flow based on recorded test data.

Finally, after extensive experimental testing, and a strict adherence to the manufactures data sheet in calculating the BPV performance, it was still found the that modeled back pressure valve did not respond according to the test data. Specifically the back pressure valve model showed almost no sensitivity to the changes in flow rate and composition that occur during a real or simulated vehicle shift. During
these shifts, the large consumption of oxygen is momentarily stopped, leading to a larger mass of gas passing through the back pressure valve, coupled with a change in the gas composition. Despite several attempts to address this, the simplest method to allow the model to reflect the actual performance was to introduce a final tunable parameter that causes the back pressure valve to simply be more restrictive than the data sheet shows.

This new parameter is called $K_{BPV}$ and it is used to modify the total mass flow rate from the back pressure valve as follows.

$$W_{BPV, corrected} = K_{BPV}W_{BPV, Model}$$ (3.48)

The reason this parameter needs to be adjusted could be one of many. The valve manufacturer’s data sheet is provided for a SG of 0.6, and only provides correction factors for gases with much higher specific gravities. The SG of the gases flowing through the BB2 BPV is typically well below 0.6, much closer to 0.35. Perhaps the valve responds significantly differently at these flow rates, especially considering the valve relies on a pitot tube to maintain a relatively even pressure over a wide range of flow.

A second reason for the valve performance not matching the test data may be partly due to some dynamic response of the valve. The valve has an internal spring, and a pitot tube which creates a vacuum on the back side of a diaphragm. This may lead to some dynamics that the static model is not capable of capturing. Without extensive testing of the valve on a test stand under a variety of two-phase flows, and a variety of gas specific gravities, and under transient operations, it will be impossible to fully characterize the performance of the valve.
Figure 3.12: The calculations involved in creating the new back pressure valve curves
3.6 Laminar Flow Calculation of Pressure Drop

This section provides the equations used to calculate the laminar flow pressure drop for a single phase gas in the channels, with no reaction considered. These equations are based on the sample calculations for laminar flow pressure drop provided in [45]. The constants used in the evaluation of the equations in this section are provided in Tab. 3.1.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>$P$</td>
<td>2.4</td>
<td>bar</td>
</tr>
<tr>
<td>Oxygen Viscosity</td>
<td>$\mu_{O_2}$</td>
<td>22.89e-6</td>
<td>$N - s/m^2$</td>
</tr>
<tr>
<td>Helium Viscosity</td>
<td>$\mu_{He}$</td>
<td>22.32e-6</td>
<td>$N - s/m^2$</td>
</tr>
<tr>
<td>Vapor Viscosity</td>
<td>$\mu_V$</td>
<td>13.00e-6</td>
<td>$N - s/m^2$</td>
</tr>
<tr>
<td>Current</td>
<td>$I$</td>
<td>420</td>
<td>amps</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T_{stack}$</td>
<td>70</td>
<td>$^\circ C$</td>
</tr>
<tr>
<td>Stoich Ratio</td>
<td>$\lambda_{O_2}$</td>
<td>1.7</td>
<td></td>
</tr>
<tr>
<td>Number of Cells</td>
<td>$N_{cell}$</td>
<td>960</td>
<td></td>
</tr>
<tr>
<td>Number of Channels</td>
<td>$N_{ch}$</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>Channel Width</td>
<td>$w_{ch}$</td>
<td>1</td>
<td>mm</td>
</tr>
<tr>
<td>Channel Height</td>
<td>$h_{ch}$</td>
<td>1</td>
<td>mm</td>
</tr>
<tr>
<td>Channel Length</td>
<td>$L$</td>
<td>0.67</td>
<td>m</td>
</tr>
</tbody>
</table>

Table 3.1: Inputs used in sample laminar flow pressure drop calculations.

First the saturation pressure of the gas must be calculated based on the pressure and temperature. The sample calculation here will be done around a temperature of 2.4 Bar, and 70$^\circ C$. The equation for saturation pressure is shown in Eq. 3.8.

Next the density of the gas entering the channel must be calculated. The calculations here will assume fully saturated heliox, and the equation for the density as
Calculation of the viscosity of the mixture is made slightly more complicated due to the fact the BB2 uses a nonstandard mixture of gases, heliox, for which a published viscosity is not available. Equations provided in [45] can be used to calculate the viscosity of any mixture of gases and are shown below. The viscosity of the mixture relies on both the mass fraction of each component, $x_i$, as well as a dimensionless parameter $\Phi_{ij}$.

\[
\mu_{\text{mix}} = \frac{1}{N} \sum_{i=1}^{N} x_i \mu_i \frac{1}{1} \sum_{j=1}^{N} x_j \Phi_{ij}
\]  

(3.50)

The equation for $\Phi_{ij}$ must be calculated for each possible combination of gases for the total of $N$ individual species. In the calculation of $\Phi_{ij}$, $M_i$ and $M_j$ refer to the molar masses of species i and j.

\[
\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j}\right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} + \left(\frac{M_i}{M_j}\right)^{1/4}\right]^2
\]

(3.51)

The stack flow rate can be calculated based on the current draw and the Oxygen stoich ratio, $\lambda_{O_2}$. Alternatively for the BB2 it could be read from the data recorded by the flow rates from the mass flow controllers.

\[
Q_{\text{stack}} = \frac{I}{4F} \left(\frac{\lambda_{O_2}}{r_{O_2}}\right) \frac{RT_{\text{stack}}}{P_{in} - \phi P_{sat}}
\]

(3.52)

With the known volumetric flow rate entering the stack, it is quite easy to calculate the flow rate through a single channel, and then calculate the velocity of the flow in the channel. The required information is the number of cells $N_{\text{cells}}$, the
number of channels per cell, \( N_{ch} \), and the area of each channel, \( A_{ch} \).

\[
v_{ch} = \frac{Q_{stack}}{N_{cell} N_{ch} A_{ch}} \tag{3.53}
\]

For a rectangular cross sectioned channel, the hydraulic diameter can be calculated based on the channel geometry.

\[
D_h = \frac{2w_{ch}d_{ch}}{w_{ch} + h_{ch}} \tag{3.54}
\]

With velocity and hydraulic diameter known, the Reynolds number can be calculated.

\[
Re = \frac{\rho v_{ch} D_h}{\mu} \tag{3.55}
\]

With the Reynolds number, and known relationship for rectangular flow channels, the friction factor can be estimated.

\[
f \approx \frac{56}{Re} \tag{3.56}
\]

Finally the pressure drop can be calculated with the following equation.

\[
\Delta P = f \frac{L}{D_h} \frac{v^2}{2} \tag{3.57}
\]

Table 3.2 shows the calculated values for each equation listed above. The final result shows that the laminar flow pressure drop along the channel would be quite small, .0037 bar, or 3.7 mbar. This turns out to be quite insignificant compared to the total stack pressure drop that is recorded during testing, which varies from .2 to .3 bar (200-300 mbar).

### 3.7 Discretized Laminar Flow Model Development

The laminar flow equations detailed previously are for a non-reacting fuel cell channel and ignore product water development. In order to consider the reaction
Table 3.2: Results of a sample laminar flow pressure drop.

<table>
<thead>
<tr>
<th>Eqn. #</th>
<th>Variable</th>
<th>Result</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.49</td>
<td>( \rho )</td>
<td>1.30</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td>3.50</td>
<td>( \mu_{mix} )</td>
<td>1.13e-5</td>
<td>N·s/m(^2)</td>
</tr>
<tr>
<td>3.52</td>
<td>( Q_{stack} )</td>
<td>.0596</td>
<td>m(^3)/s</td>
</tr>
<tr>
<td>3.53</td>
<td>( v_{ch} )</td>
<td>1.72</td>
<td>m/s</td>
</tr>
<tr>
<td>3.54</td>
<td>( D_h )</td>
<td>1.00e-3</td>
<td>m</td>
</tr>
<tr>
<td>3.55</td>
<td>( Re )</td>
<td>198</td>
<td></td>
</tr>
<tr>
<td>3.56</td>
<td>( f )</td>
<td>.2815</td>
<td></td>
</tr>
<tr>
<td>3.57</td>
<td>( \Delta P )</td>
<td>0.0037</td>
<td>Bar</td>
</tr>
</tbody>
</table>

of the gases down the length of the channel, and to deal with the product water creation, a discretized laminar flow model has been developed. The model will not predict the total stack pressure drop, as the sample calculations above show the pressure drop to be orders of magnitude below the recorded pressure drop. Instead the purpose of the model is to provide a relation between the gas flow through the channel, the liquid water production, and the liquid water exiting flow rate.

This model is not trying to explain the actual phenomena of water build up in the channel in a microscopic way. It is known that the flows can be composed of water droplets that form on the hydrophobic GDL, and are dispersed by the air flow. Instead, the hope is that a simplified model of a single channel can be used to predict the overall performance of the entire fuel cell stack combined. In fact, if the water were to form in a perfect film on the GDL, the fuel cell would not work, because it would completely prevent the oxygen from accessing the MEA so the reaction may occur. However, some studies have shown that a film may build along the channel walls, so the simplified model will hopefully capture the gross total of the water dynamics of the actual cell.
First the basic equations of a single discretization are developed. Then the discretization can be combined into a complete cathode model.

### 3.7.1 Development of the equations for a single discretization

The equations developed in this section are based on the laminar flow theory for a fluid between plates of infinite width\(^{[69]}\). The flow equations are based on the assumption of fully developed internal incompressible viscous flow.

![Figure 3.13: Diagram showing the dimensions for laminar flow equation development.](image)

It is assumed that in the channels of the fuel cell there will be two separate regions of fluid flow, the gas and liquid flow, as shown in Fig. 3.13. The gas is
treated as a fluid because of the incompressible flow assumption. Also shown in Fig. 3.13 is the nomenclature used for the gas and liquid regions. The equations for each separate fluid are derived based on two different coordinate systems, with $y = 0$ starting at the bottom of the channel on the liquid side with positive up, and $Y = 0$ starting at the top of the channel on the gas side with positive facing down. It is assumed that the liquid has a height of $h$, and the gas has a height of $H$, and the sum of the two would be the total distance between the plates, $w$.

The gas viscosity is given by the symbol $\mu_g$ and the liquid viscosity is given by $\mu_L$. The velocity of the gas at any position in $Y$ is given by $U_g$ and the velocity of the liquid at any position $y$ is given by $u_L$. At the interface between the gases the velocity is equal and given by $V$, and the shear stress is also equal and given by $\tau_{yx}$.

From [69] the velocity of the lower liquid is given by Eqn 3.58.

$$u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_{1L}}{\mu_L} y + c_{2L} \tag{3.58}$$

The velocity at the bottom plate is assumed to be 0, and the velocity at the interface is $V$. This defines two boundary conditions. When $y = 0$, $u_L = 0$, and when $y = h$, $u_L = V$. Applying the first boundary condition results in $c_{1L} = 0$. The second boundary condition is then applied, and $c_{2L}$ is replaced with simply $c_L$ in Eqn. 3.59.

$$V = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h \tag{3.59}$$

Similarly, for the gas, the generic velocity equation is given by Eqn. 3.60

$$U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_{1g}}{\mu_g} Y + c_{2g} \tag{3.60}$$

Similar assumptions provide the boundary conditions. When $Y = 0$, $U_g = 0$, and when $Y = H$, $U_g = V$. Applying the first boundary condition results in $c_{1g} = 0$. 

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The second boundary condition is then applied, and $c_{2g}$ is replaced with simply $c_g$ in Eqn. 3.61

$$V = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{c_g}{\mu_g} H$$ (3.61)

Now there are two equations for $V$ that rely on two unknown constants, $c_L$ and $c_g$. Next the shear stress is used to provide a 3rd and 4th equation. For a Newtonian fluid, the shear stress is given by Eqn. 3.62.

$$\tau_{yx} = \mu_L \left( \frac{du_L}{dy} \right)$$ (3.62)

The velocity of the liquid is inserted into the above equation. When the derivative is taken, and the equation is evaluated at $y = h$, the shear stress equation for the liquid is the result.

$$\tau_{yx} \big|_{y=h} = \left( \frac{\partial p}{\partial x} \right) h + c_L$$ (3.63)

Similarly, when the gas velocity equation is inserted into the shear stress equation, and its derivative taken, and evaluated at $Y = H$, the shear stress for the gas is the result.

$$\tau_{yx} \big|_{Y=H} = \left( \frac{\partial p}{\partial x} \right) H + c_g$$ (3.64)

If Eqn.’s 3.63 and 3.64 are set equal to each other, a 3rd equation is introduced without introducing any new unknowns.

$$\left( \frac{\partial p}{\partial x} \right) h + c_L = \left( \frac{\partial p}{\partial x} \right) H + c_g$$ (3.65)

Thus with Eqn’s 3.59, 3.61, and 3.65 there are 3 equations with 3 unknowns of $V$, $c_L$, and $c_V$. Complete derivation can be seen in the appendix.

Using the 3 equations, analytical solutions for $c_L$ and $c_g$ can be shown to be as follows. In addition, two new terms $CC_L$ and $CC_g$ will be introduced to simply the
With the analytical solutions for \( c_L \) and \( c_g \) from Eqn’s 3.66 and 3.67, the complete equations for the velocity as a function of \( y \) or \( Y \) can be found.

\[
\begin{align*}
u_L &= \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2} \frac{h^2}{\mu_L} y^2 + \frac{CC_L}{\mu_L} y \right] \\
U_g &= \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2} \frac{h^2}{\mu_g} Y^2 + \frac{CC_g}{\mu_g} Y \right]
\end{align*}
\]

Equations 3.68 and 3.69 give the velocity profile for the gas and liquid flow based on the assumptions provided at the beginning of this section. Next the velocity profile can be integrated to determine the volumetric flow rate for both the gas and the liquid. The generic equation for volumetric flow rate of a fluid field is given below.

\[
Q = \int_A \vec{V} \cdot \vec{dA}
\]

Assuming one dimensional fluid flow, and a channel width \( w \), instead of infinite parallel plates, the volumetric equation for the liquid portion can be written in more general terms as follows.

\[
\frac{Q_L}{w} = \int_0^h \nu_L \, dy
\]

The full integral can be calculated and evaluated to find the equation for the volumetric flow rate of the liquid.

\[
\frac{Q_L}{w} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6} \frac{h^3}{\mu_L} + \frac{CC_L}{2 \mu_L} h^2 \right]
\]
It can similarly be shown that the gas volumetric flow rate is given by the following equation.

\[
\frac{Q_g}{w} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6 \mu_g} H^3 + \frac{CC_g}{2 \mu_g} H^2 \right]
\]

(3.73)

The volumetric flow rate equations for the liquid and gas flows have been derived. Next the equations can be solved to get the mass flow rate, if the assumption of a constant upstream and down stream pressure are made. Figure 3.14 shows the relevant dimension of the channel. If there is a constant pressure at the inlet \( P_1 \) and the outlet \( P_2 \) of the channel then the partial derivative can be rewritten as follows where \( L_{chan} \) is the total length of the fuel cell channel and \( n_d \) is the number of discretizations that will be used.

\[
\frac{\partial p}{\partial x} = \frac{P_1 - P_2}{l} = \frac{P_1 - P_2}{L_{chan}/n_d}
\]

(3.74)

Figure 3.14: Diagram of dimensions used for laminar flow equation development.
Replacing the partial derivative, the final expression for the volumetric flow rates of the liquid and gas is shown below.

\[
Q_L = w \left( \frac{P_1 - P_2}{L_{\text{chan}}/n_d} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L h^2}{2\mu_L} \right] \\
(3.75)
\]

\[
Q_g = w \left( \frac{P_1 - P_2}{L_{\text{chan}}/n_d} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g H^2}{2\mu_g} \right] \\
(3.76)
\]

The final step is to convert the volumetric flow equation into the mass flow rate equation, which will be used in the larger model. Since the flow is incompressible, the mass flow rate is simply the density times the volumetric flow rate. Therefore the mass flow rate of the liquid and gas can be written as follows.

\[
\dot{m}_L = \rho_L w \left( \frac{P_1 - P_2}{L_{\text{chan}}/n_d} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L h^2}{2\mu_L} \right] \\
(3.77)
\]

\[
\dot{m}_g = \rho_g w \left( \frac{P_1 - P_2}{L_{\text{chan}}/n_d} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g H^2}{2\mu_g} \right] \\
(3.78)
\]

### 3.7.2 Combining the discretization into a complete channel model

In the previous section equations for the mass flow rates of liquid and gas in a channel were derived. The derivation was based on the assumptions of incompressible laminar flow. The final equations give the mass flow rate out of a theoretical single channel with a constant pressure drop, and a known liquid height.

This model will now be combined in series to create a representation of the entire fuel cell channel. In the actual channel, gases will be reacted down the length of the channel, and water will be created. The height of the liquid in the channel will be changing in time. The model will be developed so that there are \( n \) discretizations, which can be varied as required. Figure 3.15 shows the physical representation of 3 separate discretizations linked together.
Figure 3.15 shows that each discretization will have its own inlet flow and outlet flow of liquid water. Liquid water will also be added to each discretization due to the reaction electro chemistry. It will be assumed all the water will be generated in the liquid form and added directly to the water puddle. It is also assumed that the current density along the length of the channel is equally distributed. By tracking the mass of the liquid water, the height of the water puddle $h$ can be determined for each discretization. It will be assumed that there is no evaporation of water because the gas stream is already fully saturated, and condensation will be ignored due to the small reduction in volume between each discretization.

As shown in Fig. 3.15 each discretization will have an inlet flow of gas and an outlet flow of gas. The subscript g in the figure refers to the mixture of gases, but in each volume the mass of each individual component of gas will be tracked separately. This is necessary because the oxygen will be reacting based on the electrochemistry of the reaction. With the liquid height known from the water mass balance, the gas
volume of the discretization is known, and the pressure of the discretization $P_n$ can be determined.

Equations 3.77 and 3.78 can be used to calculate the exiting flow rate of each individual discretization if the inlet and outlet pressures are known. Since the pressure is directly related to the mass of the gases in each discretization, the outlet flow rate will be based on the time dependent pressure of the current discretization and the subsequent discretization. In this respect Eqn’s 3.77 and 3.78 can be rewritten as follows, using the notation shown in Fig. 3.15.

$$W_{L,\text{out},n} = \rho_L w \left( \frac{P_n - P_{n+1}}{L_{\text{chan}/n}} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L}{2\mu_L} h^2 \right] \quad (3.79)$$

$$W_{g,\text{out},n} = \rho_g w \left( \frac{P_n - P_{n+1}}{L_{\text{chan}/n}} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g}{2\mu_g} H^2 \right] \quad (3.80)$$

A block diagram showing how the calculations are made is provided in Fig. 3.16. The calculations are broken up into a few different blocks. Inputs to the model are inlet flow rates from the previous discretization, the pressure of the subsequent discretization, and the reacted and generated terms from the electrochemistry. The equations for each block, as well as the electrochemistry will be detailed here.

**Gas Mass Balance Block**

The equations used in the gas mass balance block do not differ much at all from the equations used in the control oriented model development. The mass of each component of gas is calculated based on the inlet and outlet flow rates of the gases, and for the oxygen the reacted term is considered from the electrochemistry.

$$\frac{dm_{O_2,n}}{dt} = W_{O_2,\text{in},n} - W_{O_2,\text{out},n} - W_{O_2,\text{reacted},n} = W_{O_2,\text{out},n-1} - W_{O_2,\text{out},n} - W_{O_2,\text{reacted},n} \quad (3.81)$$

77
Water Mass Balance Block

Similarly the mass of the liquid water in each discretization is also tracked with a simple mass balance that includes the inlet flow from the previous block, and the outlet flow which is calculated within the discretization. The addition of liquid water is also an input due to the electrochemistry. The liquid water equation here is different than in the control model development, because it is assumed there is no interaction between the liquid and gas phases due to the saturated inlet stream.
and negligible change in volume that would lead to condensation.

\[
\frac{dm_{L,n}}{dt} = W_{L,\text{in},n} - W_{L,\text{out},n} + W_{L,\text{generated},n} = W_{L,\text{out},n-1} - W_{L,\text{out},n} + W_{L,\text{generated},n}
\]  

(3.84)

**Generation and Consumption Terms**

In Fig. 3.16 the electrochemical reaction terms are shown as inputs. The equations for the electrochemical reaction are nearly identical to the equation already provided in the control model, except the current must be divided by the number of discretizations used \( n_d \), because it is assumed that the current is equally distributed.

\[
W_{O_2,\text{reacted},n} = M_{O_2} \times \frac{nI_{st}}{n_d4F}
\]  

(3.85)

\[
W_{L,\text{generated},n} = M_v \times \frac{nI_{st}}{n_d2F}
\]  

(3.86)

**Height of Water Puddle and Gas Volume**

The block that calculates the height of the water puddle contains a fairly simple equation. Since the water has a constant density, and its mass is known, the determination of the water puddle height can be determined based on simple geometric calculations. The height of the gas side \( H \) can be determined as well. Finally, the volume available for the gas can be calculated.

\[
h = \frac{m_{w,n}}{wpL_{\text{chan}}n_d}
\]  

(3.87)

\[
H = w - h
\]  

(3.88)

\[
V_g = hwL_{\text{chan}}n_d
\]  

(3.89)
Gas Pressure Calculations

The calculation of the gas pressure of the components is calculated exactly as it was in the control model, but uses the new volume available for gas based on the height of the water. The equation is presented for a general gas component i, but equations for each component are calculated separately. The total pressure is the sum of the partial pressures of each gas component.

\[ p_{i,n} = \frac{m_{i,n} R_i T_{st}}{V_g} \quad (3.90) \]

Water and Gas Outlet Flow rate

The equations for the gas and water outlet flow rate were previously shown in Eqn’s 3.79 and 3.80. The liquid outlet mass flow rate is fed back to the mass balance block, and is also fed out as the input to the next subsequent discretization. The gas outlet flow rate is calculated, but is based on the instantaneous gas density and Eqn. 3.80 only gives the output for the total gas mixture. Therefore the details of calculating the independent outlet flows of each component must be provided.

First the density at any instant in time is simply the mass of all gas components divided by the volume of the gas.

\[ \rho_g = \frac{m_{O_2,n} + m_{He,n} + m_{V,n}}{V_g} \quad (3.91) \]

The exit flow rate of each component will then be based on the mass fraction of the gas mixture in the discretization. In the equation below the subscript i refers to any of the three gas components of the mixture.

\[ X_{i,n} = \frac{m_{i,n}}{m_{g,n}} \quad (3.92) \]
Finally it is possible to calculate the cathode outlet flow rates for each individual species from the outlet flow rate and the mass fraction, as shown in below.

\[ W_{i,\text{out},n} = X_i W_{g,\text{out},n} \]  \hspace{1cm} (3.93)

**Interconnecting the Discretizations**

The detailed equations inside each discretization have been provided. Next the details of how the discretized models should be interconnected, and interface with the rest of the model are provided. The total model is broken up into three separate model sections, as shown in Fig. 3.17. The three model sections are the inlet manifold volume, the discretized model, and the exhaust manifold volume.

![Figure 3.17: Block Diagram of total system with the discretized model integrated.](image)

The inlet manifold is treated as a separate control volume before the gases enter the distributed model. The equations used to govern the volume need not be
detailed, as they are simple mass balance and pressure calculations that have been
detailed many times in this chapter. The generation and reaction terms are not
used in the inlet manifold mass balance because there is clearly no reaction or con-
sumption occurring in the manifold. A resistance must be defined between the inlet
manifold volume and the exhaust manifold. This flow resistance will be detailed in
the following section. What is important to detail here is that the pressure from the
first discretization must be fed back to the inlet manifold volume to determine the
flow into the first discretization.

The exhaust manifold model used in the total model is the two phase exhaust
system model detailed in Section 3.5. The pressure from the exhaust manifold must
be fed back to the final discretization of the model.

Figure 3.18: Block Diagram showing the interconnection discretizations inside the
discretized block.

Figure 3.18 shows the details of the interconnection of a sample with three
lumped models. In the digram, the terms $W_{out}$ will refer to flow of both the water
and gas, which are tracked separately. As the diagram shows, and as discussed above, the first discretization will output a pressure that will be fed back to the inlet manifold volume. The pressure of the exhaust manifold must also be fed back into the final discretization of the model, so that the outlet flow rate from the final discretization may be calculated. The outlet flow rate of the final discretization is the total cathode outlet flow rate that goes into the exhaust manifold volume.

### 3.7.3 Upstream Resistance

In order for the discretized model to work, an inlet flow rate must be defined for the first discretization. While the outlet flow rate of the mass flow controllers could possibly be used simply as an input to the discretization, this would ignore the inlet volume, which consists of fairly large tubing as well as a significant volume for the humidifier. To be sure these dynamics are accounted for, the inlet volume must be considered.

To generate the outlet flow from the inlet manifold, the simple linearized resistance used in the control model will be used to represent the lumped flow resistance between the inlet manifold and the start of the fuel cell channels. Since the resistance at this point in the fuel cell will only have saturated heliox flow, its equations for the outlet flow of each gas are exactly similar to those detailed for the control level model. The total outlet flow rate for the gas mixture is calculated from the pressure difference between the inlet manifold and the first discretization.

\[ W_{im,\text{out}} = K_{US}(P_{im} - P_{1^{\text{st Disc}}}) \]  

(3.94)
Next the mass fraction split of the gases is used to determine the outlet flow rate of each component $i$.

\[
m_{total,im} = m_{O_2,im} + m_{He,im} + m_{v,im}
\]

(3.95)

\[
X_{i,im} = \frac{m_{i,im}}{m_{total,im}}
\]

(3.96)

\[
W_{i,im} = X_{i,im}W_{im,out}
\]

(3.97)

### 3.7.4 Downstream Stack Resistance Model

Through model development and validation, it was found that using only the inlet manifold resistance, and the discretized model, the pressure drop characteristics of the system were not accurately captured. Inspection of the airflow path reveals some insight as to why this might occur. Figures 3.19 and 3.20 give a representation of how the cathode gas flows through the complete stack.
Figure 3.19: The stack manifold distributes gas flow to the individual cell rows.
Figure 3.20: The air flow path through a cell row is distributed to each cell, and then to each cell channel.
The gas first enters a manifold, which directs the gas to each of the 6 cell rows. The gas then must travel down a runner within each cell row, where it enters the channels. The gas encounters significant restrictions from the runner into the channels as it is separated into each channel. This is in addition to the resistance it encounters through the manifold and down the length of the runners.

It's important to note here, that the gas on the upstream side encountering these restrictions is of a constant composition, that of fully humidified heliox. This explains why the resistance of the stack shows no change as more and more water exits from the stack when only an upstream resistance is considered. It is also shown in the results section that the simple laminar flow resistance across the stack is practically negligible, meaning that the flow resistance that is encountered is mainly due to effects outside of the flow channels.

Looking now at the exit path, the gas faces a significant restriction as well. The gas must recombine at the end of the channel and exit into the runner. Then the gases from each cell row runner are recombined in the manifold to a single outlet. Physically it makes sense that the exit restriction is likely smaller than the inlet restriction, because the gas does not have to be separated into each channel. The downstream resistance should be similar to, but have less of a magnitude than the inlet resistance. However, a key difference to this restriction is that the composition can vary greatly. The composition will change depending on weather or not oxygen is being consumed due to current draw, and its composition will change depending on the rate at which liquid water exits the cathode channels.

The flow in the exiting portion of the fuel cell will be treated similar to the flow in the two phase flow exhaust model. It is assumed that there are no methods for
water to be accumulated in the exit flow path, and the water droplets are perfectly
dispersed within the gas mixture. The Cathode Exit (CE) is given a volume equal
to the volume of one discretization of the channel model. The exiting mass flow
rate from the cathode exit is determined by the pressure differential between the
exhaust manifold and cathode exit pressure.

\[ W_{CE,out} = K_{DS} (P_{CE} - P_{em}) \] (3.98)

The exiting mass flow rate of each component is calculated based on the to-
tal mass flow rate calculated from the resistance. The liquid water is treated as
component of the mixture.

\[ m_{total, CE} = m_{O_2, CE} + m_{He, CE} + m_{v, CE} + m_{L, CE} \] (3.99)

\[ X_{i, CE} = \frac{m_{i, CE}}{m_{total, CE}} \] (3.100)

\[ W_{i, CE, out} = X_{i, CE} W_{CE, out} \] (3.101)

A block for this secondary stack resistance can be built according to the equations
in this section and implemented in the complete model between the distributed
cathode model and the exhaust manifold volume. Figure 3.21 shows how this is
implemented in the overall model.

Using Total Mass of the Two-Phase Mixture vs. a Variable Resistance

This is a simplified method of dealing with the liquid flow through a restriction,
by adding the mass of the liquid as an equal component to the gas mixture. At first
this does not appear to be the most theoretically appropriate method of dealing with
two phase flow, because with two phase flow the gas and liquid will not always flow
at the same rate. However, if the assumption of a homogeneous two-phase mixture
Figure 3.21: The downstream resistance implemented in the total model.

is used, another method of dealing with the water would instead be to make the flow resistance more restrictive proportional to the mass fraction of water. It can be shown mathematically that these two methods will result in the same solution. Below the subscripts \(g\) will simply refer to the gas mixture, which could have many components.

According to the methods used in this work, the flow rate of the total mixture of gas and liquid is proportional to the pressure difference for a linearized case.

\[
W_{total} = k\Delta P
\]  

The preferred method is to make the only the gas portion of the flow rate proportional to the pressure difference. In this case we will make the restriction proportional to the gas mass fraction. The lower the mass fraction of gas is, with the
same delta P, the less gas flow rate there would be.

\[ W_g = k X_g \Delta P \]  \hspace{1cm} (3.103)

Assuming the mixture is homogeneous, the total flow rate will be the sum of the gas and liquid portions, and the liquid portion will be the total times the liquid mass fraction.

\[ W_{total} = W_g + W_L = W_g + X_L W_{total} \] \hspace{1cm} (3.104)

The above equation can be solved for \( W_g \), and set equal to Eqn. 3.103

\[ W_g = W_{total} - X_L W_{total} = W_{total} [1 - X_L] = k X_g \Delta P \] \hspace{1cm} (3.105)

Next, by definition, the sum of the liquid mass fraction and gas mass fraction are equal to 1.

\[ 1 = X_g + X_L \] \hspace{1cm} (3.106)

Equation 3.106 can be solved for \( X_g \) and inserted into Eqn. 3.105.

\[ W_{total} [1 - X_L] = k [1 - X_L] \Delta P \] \hspace{1cm} (3.107)

The result is that Eqn. 3.107 is equal to Eqn. 3.102, showing that the two methods provide equal results.

\textbf{3.7.5 Downstream Resistance Using a Two Phase Resistance Model}

The method of adding the mass of the liquid to the total mass flow rate determined by the resistance is a rather ad-hoc method of accounting for the water droplets entrained in the stream. In order to explore a method to better describe the flow resistance with two phases, a text on two-phase flow was consulted.
In [70] a section is written on pressure drop in a flow restriction for steady state, homogeneous, two phase flow. The section details the importance of pressure drop at restrictions, but states that the integrated momentum and kinetic energy before and after the restriction cannot be calculated analytically. Therefore semi empirical or empirical models are often used. The recommended equation from [70] for two phase flow through a restriction is given below.

$$\Delta p_c = \frac{A_2^2 G^2}{2 g_c A_1^2} \left[ \left( \frac{1}{A_{VC}} - 1 \right)^2 \left( 1 - \frac{A_1}{A_2} \right)^2 \right] \left[ \frac{X}{\rho_G} - \frac{(1 - X)}{\rho_L} \right]$$

(3.108)

In Eqn. 3.108, \(G\) is the mass flux, which is the mass flow rate per unit of area. \(X\) is weight percent of the steam, or the steam mass fraction. \(\rho_G\) and \(\rho_L\) refer to the gas and liquid densities respectively, and \(g_c\) is a gravimetric conversion factor because the units in [70] are based in English units, not SI. The remaining parts of the equation, \(A_1\), \(A_2\) and \(A_{VC}\) refer to the upstream area, downstream area, and the area of the vena contracta respectively.

For implementation into the fuel cell, we are looking for a way to lump all the downstream flow resistances into a single resistance that is sensitive to the composition of the two phase flow. In that respect, the equation above will be rewritten, grouping the terms that are essentially constants, to a single flow resistance, \(K_{DS}\). This resistance will have to be calibrated from empirical results.

$$\Delta p_c = \dot{m}^2 K_{DS} \left[ \frac{X}{\rho_G} - \frac{(1 - X)}{\rho_L} \right]$$

(3.109)

### 3.7.6 Discretized Model with Slip Velocity

The discretized model was developed using fully developed laminar flow calculations to derive the theoretical velocity profile of a gas flowing over a liquid. The
The model assumes that there is a film of water attached to the bottom side of the cathode flow channel. Much research has been published showing that the water does not actually build up and exit in such a smooth controlled fashion. Instead the water can actually develop into droplets that stay attached to hydrophobic GDL, until their mass is large enough to restrict the flow to a point where the velocity of the gas detaches the droplet and it flows out of the channel. Many other visualization studies show that the liquid also attaches to the walls, and even the top of the channel, not simply along the bottom of the channel.

The purpose of developing the discretized model was not to use the model to show how water really behaves in the cell channel. Instead the purpose was to derive a physically based model, that might at least capture the dynamics related to water buildup, and its eventual steady state exit rate from the channel. To this respect, the model derived provided no empirically tunable method to adjust the model to reflect experimental results should the model not correspond to physical reality.

To consider a tunable parameter that might reflect empirical results, the idea of including a slip parameter between the liquid and gas velocities is evaluated. Since it is most likely that the gas will be traveling faster than the liquid, the slip equation is written as follows.

\[ V_L = \alpha V_g \]  

(3.110)

The variable \( \alpha \) is introduced so that the liquid velocity may be only a portion of the gas velocity.

The full derivation of the final equations is shown in the appendix. Only the final equations will be shown here. The expression for the volumetric flow rate of the liquid remains unchanged, but the constant \( CC_L \) shows the influence of the addition
of slip.

\[
\frac{Q_L}{w} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L}{2\mu_L} h^2 \right] \tag{3.111}
\]

\[
CC_L = \frac{\alpha H h}{\mu_g} - \frac{h^2}{2\mu_L} - \frac{\alpha H^2}{2\mu_g} \tag{3.112}
\]

Similarly, the expression for the gas volumetric flow rate remains unchanged, while the constant \( CC_g \) reflects the new addition of slip.

\[
\frac{Q_g}{w} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g}{2\mu_g} H^2 \right] \tag{3.113}
\]

\[
CC_g = \frac{\frac{H h}{\mu_L} + \frac{h^2}{2\mu_L} + \frac{\alpha H^2}{2\mu_g}}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]} \tag{3.114}
\]

Because the slip does not show up directly in the volumetric flow rate equation, but instead shows up inside the constants \( CC_L \) and \( CC_G \), the mass flow rates equations 3.78 and 3.77 also remain unchanged, so they do not need to be repeated here.

### 3.8 Conclusion

This chapter has provided an overview of the modeling techniques applied to the BB2 system. This started by adapting the commonly referenced control model from [60], which does not consider the effects of liquid water. A simple modification to this model was proposed that uses a simple method to account for the combined liquid and gas flows. Next, laminar flow theory was used to create a discretized model that can be used to help predict the water outlet flow properties of the stack. Finally the model was refined by adding an additional downstream resistance, using both a simple method, and a method involving equations used for two-phase flow.
CHAPTER 4

Testing Methodology and System Performance Optimization

Optimization of the performance of this complex fuel cell system required a large amount of testing and tuning. This chapter details the testing and the methodology that lead to the successful performance of the BB2 race vehicle. Initial testing was conducted to verify the theoretical capability of a PRV system to protect the fuel cell modules from over pressurizing. This was followed by performance testing which initially exposed a major cell imbalance between FCM A and FCM B. Once this cell imbalance was resolved, final testing and tuning of the PRV’s and BPV’s was completed to reach maximum performance by operating as close as possible to the pressure design limits of the stack. In addition, a few tests were conducted to measure the rate at which liquid water exits the stack to aid in the validation of the discretized model developed in Chapter 3.

4.1 Cathode PRV Implementation

Analysis of test data from the 2007 and 2008 race season lead to the conclusion that the mass flow controllers were capable of flowing damaging amounts of heliox to the cathode of the fuel cell system. A simple ideal gas model detailed in the work
of Bork[17] was able to show this problem. It was found that if the MFC were to get stuck in a full open position, the amount of inlet flow to the cathode would be so high, that the flow resistance across the stack itself could lead to damaging pressure levels upstream of the stack.

Under ideal conditions, the mass flow controller should never reach these damaging flow levels. However the MFC that was supplying FCM B was known to have poor control issues when transitioning from idle flow rate to full flow rate for racing. As seen in Fig. 4.1, the flow rate overshoots, and actually saturates the flow sensor that is built into the mass flow controller. This poorly performing mass flow controller was replaced, but since a full open failure was still a possibility, testing was required to verify that PRV’s would be an acceptable solution.

4.1.1 PRV Testing

The most robust test would be to simulate the damaging input flow rates into an operational system to see if the PRVs would be capable of limiting the pressure. However, if the PRVs were incapable of this, then it would be possible to again damage the fuel cell stack, which is a dangerous and costly risk to take.

Instead of running the risk of stack damage, the available test data was analyzed to determine a normal operating flow rate, and associated pressure drop. Then a large ball valve was adjusted to provide a similar flow resistance to the stack. The test setup is shown in Fig. 4.2. The downstream pressure was simulated using the same BPV’s that were used in the race vehicle. Upstream and downstream pressure sensors were installed to record the pressure transients.
Figure 4.1: Data from overpressure event.
Figure 4.2: Test setup for PRV testing.
Recreating the flow overshoot was another challenge, since it was not a consistent problem. To simulate this overshoot, the MFCs were tricked. The MFC command was given, but the supply gas was manually cut off with a ball valve. The MFCs therefore went to a fully open condition, since they had a command, but no supply gas. Then the supply ball valve was opened quickly, leading to a flow surge that repeated the conditions seen during the over pressure events. Figure 4.3 shows the recorded data inputs during a PRV test procedure.

The top plot in Fig. 4.3 shows the available tank pressure. The second plot in 4.3 shows the regulated pressure available upstream of the mass flow controller. As the figure shows, around a time of 0 seconds the available pressure shoots from 0 to 7 bar. This corresponds to when the ball valve is opened allowing heliox to the mass flow controller. The flow overshoot is well simulated because the 3rd plot in 4.3 shows that the mass flow controller command is given well before a time of 0, meaning the mass flow controller goes to a full open state when no gas is available. The 3rd plot also shows that the mass flow controller feedback signal (0-800 non dimensional units) reaches its saturated 800 unit level, and then reaches a regulated flow rate around a time of 7 seconds. During this time the inlet pressure is seen to spike around 5 bar, which would be well above the stack design limits.

4.1.2 Test Results

With the overshoot input conditions well simulated, several tests were conducted to test the robustness of the proposed PRV system. The first test was to record the baseline conditions if no PRV system were used. Then a single PRV was used, with 45 psi pressure setting. The pressure setting simply refers the pressure at which
Figure 4.3: Input data from a test of the PRV system.
the PRV begins to allow trace flow from a test setup with nitrogen as a supply gas. Next the same overshoot simulation was conducted with a 40 psi setting, and finally a test was conducted using two back pressure valves with a 40 psi setting.

Figure 4.4 shows the results of the 4 separate PRV tests. The baseline condition with no PRV system shows that the stack inlet pressure could have possibly been as high as 5.4 Bar, which is well above the design limit of 3.2 bar. The results do show that the PRV is an effective method of controlling the peak system pressure. Simply using the 45 psi setting reduces peak pressure to just over 4 bar. Reducing the setting further to 40 psi keeps the peak pressure very close to the design limit. The gain of using two PRV’s in parallel was quite minimal, and it was felt that if further reduction in peak pressure were required, it could simply be obtained by further reducing the pressure setting of a single PRV.
A single PRV was installed per FCM, as shown in Fig. 4.5. The PRV was installed between the Ballard cathode humidifier and the stack inlet manifold. This is the closest location available to the stack inlet, and provided the greatest ability to vent excess pressure in the case of a pressure spike, or overflow condition from the mass flow controller.

4.2 Load Bank Testing Methodology

To test the fuel cell system under full power, a novel test method was needed to provide the ability to focus purely on the fuel cell system and optimize its performance.

The fuel cells can be tested in the vehicle, either on the test track, or at Bonneville. However this is not a quick or easy way to test system changes. Running
the entire vehicle requires a lot of effort from the entire team to ensure the vehicle, suspension, steering, and brakes are all in working order before a test can be conducted safely. In addition, refueling is a problem at the test track, because if the vehicle runs out of fuel, it must be recovered and towed back to a fueling location. This problem is multiplied in complexity when tested at Bonneville. Long lines of other race vehicle are almost always present, meaning that half of a full day can be waisted to complete a single test.

A solution for testing the vehicle in the shop could be to use the 1000 HP dyno available at the OSU CAR. While this is an acceptable method, there are a few problems to this test methodology. First, it requires a few more people to be available to run a test, because people must be available to operate the dyno, and monitor the motor performance. The second problem is that due to the controls of the motor dyno, it is not possible to simulate transmission shifts.

4.2.1 The Load Bank

The ideal solution required a method to test just the electrical output of the fuel cell system. However, with fuel cell output exceeding 500 kW, this is no trivial load to be dissipated. The solution to this was the construction of an electrical load bank with some relatively simple to attain components. Figure 4.6 shows the setup. A fan from a decommissioned wind tunnel is powered by a 15 HP 3-phase motor to provide cooling flow. The electrical load is dissipated by 9 resistors.

The resistors are wired in parallel, with remote switches used to add them to a parallel connection one at a time. This allows the resistance of the entire setup to be lowered, and more load current can be drawn from the load bank depending
on the required test to be run. Figure 4.7 shows the load bank glowing red before the larger cooling fan was added to keep the resistors cool during an entire run. Figure 4.8 shows the resistor load bank during a run with the high power fan going. Infrared imaging shows even when the large fan is used the resistors can exceed 270 °C.

During preparation for the 2008 race season, the load bank was used to test maximum system power. In these tests, the current draw was simply brought to the highest level that the system could attain before the cells would crash due to concentration losses. In this testing the fuel cell system was capable of producing peak power near 600 kW. However these tests were quite short in duration, as each test typically resulted in a new problem found, or the test was being used to evaluate the results of a system change. Much of this work was focused on the optimization
Figure 4.7: The load bank glowing red during a high power test.

Figure 4.8: IR camera image of the resistors during a full power load bank test.
of the components in the hydrogen delivery system and are well detailed in the work of Bork [17].

4.2.2 Shifting Simulation with the Load Bank

The major breakthrough attained with the use of the load bank in preparation for the 2009 race season was through the ability to simulate full length runs from Bonneville. The goal was to simulate a full length Bonneville run to test all components for the exact duty cycle they would see. This would test the full design of the cooling system, as well identify any problems in the fuel cell system that might be a result of long duration high current draw. The initial goal was simply to achieve and hold high current draw from the fuel cells for as long as possible.

However, when the load current data from the 2008 race season was analyzed, two things were noticed that a simple high current test would not capture. First, as the vehicle is accelerating the current builds up from approximately 0 to 400 amps per module over a time span of roughly 15 seconds, no where near an instantaneous current step. The second trend was that during each shift of the transmission, the current momentarily drops to zero, and then is quickly back to full current draw. The goal of the testing was to simulate the real race condition as closely as possible in every possible way.

To mimic the race event current draw, the switching of the load bank was performed manually to roughly match the current profile of the race vehicle. Since the resistors can only be switched on in 9 discrete steps, the current ramp up cannot be smooth, but it can be approximated. To simulate the shift sequence, all the switches had to be cut simultaneously, and then ramped up to full current with in about one
Figure 4.9: A load bank current profile overlaid on a Bonneville race current profile.

second. Using a stop watch, and with a little practice, it is possible for a human operator to match the current profile with a reasonable accuracy.

Figure 4.9 shows current profiles from the race conditions in Bonneville for Modules A and B. These are labeled A Bonneville and B Bonneville. The load bank current profiles from a sample test are overlaid, and labeled A Test Stand and B Test Stand. The figure shows that with close attention to the manual control of the load bank switches, a reasonably close approximation of the race current profile can be achieved. This was a major break through for testing, as it lead to the identification
of pressure spikes during the shift that required system design changes, and much testing to control properly.

In preparation for the 2009 race season, the resistor bank was rewired because the final switch steps were reaching current levels that were unrealistic for the BB2 race conditions. In 2008 testing, all nine resistors were wired in parallel. To make the final step less dramatic for the 2009 testing, the final two resistors were wired in series, and together they were added to the parallel combination, making the final current step less dramatic. Table 4.1 compares the load bank wiring between the 2008 and 2009 setup. The table shows the resistance of each individual switch as it is added, the resulting total resistance of the bank, and an estimated current draw.

As Tab. 4.1 shows, for the 2008 setup, using switch 8 would likely draw 440 amps per module, which was above the current draws seen in the race data, and switch 9 would draw 480 amps per module, which was difficult for the fuel cells to sustain without cell voltages crashing. For the 2009 setup, switch 8 resulted in about 415 amps, which lined up better with the expectations based on the race data.

4.2.3 Load Bank Setup and Auxiliary Equipment

While the load bank provides a robust method of completing a test, a complete test does not involve a trivial amount of setup and control to complete.

Test gases are very valuable, and the tanks are refilled in the shop with pressure balancing, so the load bank tests are often a bit shorter than full duration Bonneville runs where the car was refueled with gas compressors. Because of this, it is critical that the fuel cells be pre-heated before a run. The other reason to preheat on the test stand, is that during FIA racing, the vehicle is turned around quickly between runs.
Table 4.1: Voltages of Swapped Cell Rows.

with the full support of the team, so the fuel cells remain at temperature between runs. To preheat the cells, two 220V engine heaters are used to pump warm water through the ice bath loop of the cooling system. Valves are used to shut off the normal flow path of the ice bath loop so it can be used instead as a heating circuit.

The fuel cell pumps are cycled periodically to draw heat from the heat exchanger and warm up the cells. The vehicle driver display is used to monitor the temperature of the fuel cells as they are preheated. Figure 4.10 shows the ice bath loop is at 90 °C, and the fuel cells are at 60 °C. If the fuel cell pumps are turned on the heat exchanger will equalize the temperature between the loops and add heat to the fuel cells to prepare them for the test. A full temperature warm up from ambient can take two hours or more.

Figure 4.11 shows some of the test setup required on the side of the vehicle. In the middle of the vehicle is one of the two pre-heaters hooked up to the ice bath
Figure 4.10: Vehicle display used in pre-heating sequence of the vehicle before a test.

loop. The high voltage cables that normally run from the fuel cells to the motor are directed to the load bank located near the rear of the vehicle.

More equipment is required to support the test. Figure 4.12 shows the auxiliary equipment on the left side of the vehicle. A battery cart is used to provide 12V, 24V, and 48V power to the various systems of the vehicle. This cart provides a longer duration of use than the small batteries that were used on the race vehicle, but still must be recharged periodically to ensure enough power is available to complete a test. The figure also shows the other pre-heater, and most importantly the control table.

The control table is where two or more operators will sit to run a test. Figure 4.13 shows the key components of the control table. The left computer is used to talk to the BB2 control system. It is used to fake the controller into thinking the
Figure 4.11: Test setup required on the right side of the vehicle.

Figure 4.12: Test setup required on the left side of the vehicle.
vehicle is running. The operator can command current requests to the fuel cell controller, mimicking what occurs when the driver steps on the pedal. This will increase the heliox flow rates so that current can be drawn. It can also be used to look for faults that may occur.

The second computer from the left is used to monitor the cell voltages during the run by the load bank switch operator. This gives real time feedback that may indicate the load is too high for the cells to support. The third computer from the left is used to log into the Ballard control system and monitor any addition channels that may be critical for the particular test. This software can also be used to override various commands of the automatic control system if needed. The final object on the right of the table is the switch box for the load bank and its power supply. The power supply provides the power to open the contactors that are controlled by the switches on the load bank switch box.

The final results of a successful test are the production of lots of vapor and product water when high power is being drawn. Figure 4.14 shows the author of this dissertation monitoring the cell voltages during a successful load bank test, the data of which is used in the presentation of the results.

4.3 Cell Row Imbalance Correction

This section details the correction of a cell row imbalance that was performed to equalize the performance between the two fuel cell modules. After a series of repairs, module B was under performing compared to Module A, and a swapping of cell rows between the modules allowed the current draw to be equalized so that performance could be optimized.
4.3.1 Finding the Cell Imbalance

Testing in preparation for the 2009 race season revealed that there was an imbalance in the current draw between FCM A and FCM B. When Ballard originally provided the FCMs for the BB2, they were constructed with prototype membrane technology designated MEA 9. MEA 9 is simply an internal designation referring to build level of the membrane electrode assembly. The MEA 9 had slightly better performance characteristics than a standard MEA that might have been used in the city bus program. However, they were a prototype level membrane, and were not available in large quantities.

After damaging FCM B twice in the 2008 race season due to over pressure events, Ballard had run out of sufficient quantity of MEA9s to rebuild module B completely with MEA9s. Therefore FCM B was returned to Ohio State with a mixture of MEA9s.
Figure 4.14: The steam production during a load bank test.
and the production MEA4Bs. Since the cells are connected in series in a module, the overall module polarization curve is a function of the summation of the polarization of each individual cell. The MEA4Bs have slightly lower performance than the MEA 9s and therefore a slightly lower operating voltage. This causes a problem because the FCMs are wired in parallel in the BB2 vehicle, which means they must operate at the same voltage.

Figure 4.15 highlights this problem by showing an experimentally determined polarization curve. Attention should only be paid to the highest portions of the
polarization curves for Module A and B. The points below this curve are a result of transient conditions during startup and shut down. By looking at the highest portions of the polarization plots for Modules A and B, it can be seen that if the combined system was operating at 700V, Module A would be drawing 350 Amps, while Module B would only be drawing 280 Amps. This is not really much of a concern at these current draws, but much higher current draws are required for the BB2 to perform at maximum power.

Figure 4.16 shows the current draw during a high power test of the system. It can be seen that Module A is reaching current levels near 500 amps, while Module B is only reaching around 420 amps at the same time. This causes a problem because Module A, when running at higher currents, is beginning to hit the limit of its performance by reaching the concentration losses region of its polarization curve, while Module B is not being worked to its limits.
4.3.2 Cell Row Construction

The FCMs used in the BB2 are composed of 960 cells in series. The two FCMs are then wired in parallel to provide the electricity to the vehicle. The cells in a single FCM are not all directly connected together, as this would produce a very large stack. Instead the cells are broken up into cell rows. Figure 4.17 shows the construction schematically. The electricity flows in series through the cell rows. At the end of each cell row, electrical jumpers allow the electricity to flow to the next cell row in the series. In total 6 cell rows make up the entire stack.

The entire stack can be visualized as a set of batteries connected in series, similar to almost any electrical device where the batteries are inserted next to each other, but in opposite directions. However, in a typical electric device, all the individual batteries are interchangeable. This is not true in the stack construction. For the current to flow in opposite directions between the odd and even cell rows, the gas flow routing is reversed in the cell rows. This means that between the two modules, any odd row could be swapped for an odd row, and any even row could be swapped for an even row. However, it is not possible to exchange an even row for an odd row.

The cell rows would ideally have all the same voltages, if they were all constructed using the same membrane technology. However, Module B’s cell rows were repaired with a mix of membrane technology. In addition, the repairs were not completely consistent, and completed under a short time frame, meaning they were not well documented. This results in different polarization performance for each cell row of Module B. While it is technically feasibly to swap individual cells between Module A and Module B, this is a very time consuming process that must be done with the
Figure 4.17: Internal construction of the fuel cell modules.

proper tools that only Ballard has access to. However removing and replacing an entire cell row does not require any specialized tools, and can feasibly be done in the field, *ie* in the shop at Ohio State.

### 4.3.3 Calculating The Ideal Cell Balance

To balance the current draw between the two modules, the cell rows can be swapped between module A and B to find a combination that would result in a more equal polarization performance between the two modules. To aid in determining the ideal swapping plan, polarization performance of each individual cell row was calculated. The only data source available to do this was through the cell voltage
monitor software provided by Ballard. This software is not able to produce real-time data samples, instead it had to be read manually and entered into a spreadsheet. Because of this labor-intensive process, the polarization was only examined in the medium to high current draw region.

Polarization characteristics in this region are dominated by the ohmic losses, which are predominantly linear with respect to current draw. Because of this, a linear curve fit of data collected can be reasonably made. The individual polarization curves for each cell row can be seen in Fig. 4.18. In the figure, the curve fits are shown for each individual cell row for Module A and B. In the current operating condition, Module A would typically be drawing about 430 amps, while Module B would only be drawing 370 amps. Using the curve fits, the voltage of each cell row can be estimated.
Figure 4.18: Cell row polarization curves with voltages shown with module A at 430 amps and module B at 370 amps.
Next it is assumed that a cell row swap combination could be found that would allow Module A and B to operate at the same current draw. Figure 4.19 shows the voltages of each cell row that would be obtained if the total current draw was 400 amps. From the voltages obtained from the curve fit, and knowing the restriction on even to even and odd to odd row swaps only, various combination of the cell rows can be evaluated to find a combination that results in relatively equal voltage between the two stacks. Table 4.2 lists the final choice of cell swapping, and the estimated new voltage if operated at a current of 400 amps. The table shows a very even total voltage between the two modules.
Figure 4.19: Cell row polarization curves with voltages shown with both Modules at 400 amps.
### 4.3.4 Completing the Swap and Results

The swapping of the cell rows requires that the FCMs be removed from the vehicle, and the stacks be removed from the modules. The stacks are normally oriented with the cell rows in a horizontal position, with one end attached to the gas manifold. Figure 4.20 shows the two stacks removed from the modules. The foreground of the figure shows the stack in its normal orientation with the cell rows oriented horizontally. In the background of the figure a stack has been rotated to place the rows in a vertical orientation.

With the cell rows oriented vertically, they can be detached from the gas manifold, and removed from the stack by lifting vertically. Figure 4.21 shows a stack with a single cell row removed. The cell row is seen laying flat on the table in front of the stack. The appropriate row from the other stack will be put in the same place.

With the cell rows successfully swapped, the modules were put back together, and reinstalled in the vehicle. The entire system was then tested to verify the

<table>
<thead>
<tr>
<th>Module A</th>
<th>Voltage</th>
<th>Module B</th>
<th>Voltage</th>
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</thead>
<tbody>
<tr>
<td>A1</td>
<td>107.0</td>
<td>B1</td>
<td>105.2</td>
</tr>
<tr>
<td>B6</td>
<td>110.3</td>
<td>B2</td>
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</tr>
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<td>A3</td>
<td>109.3</td>
<td>A5</td>
<td>110.3</td>
</tr>
<tr>
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<td>A4</td>
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</tr>
<tr>
<td>A6</td>
<td>110.4</td>
<td>A2</td>
<td>110.0</td>
</tr>
<tr>
<td>A</td>
<td>644.9</td>
<td>B</td>
<td>645.5</td>
</tr>
</tbody>
</table>

Table 4.2: Voltages of Swapped Cell Rows.
Figure 4.20: Both Stacks removed from the vehicle and module.

Figure 4.21: A stack with a single cell row removed.
Figure 4.22: Module polarization performance after cell swapping.

swap had equalized the performance between the two stacks. Figure 4.22 shows the polarization curves of the two modules, and Fig. 4.23 shows the current draw. As the two figures show, the performance of the two modules has been equalized, and current draw is nearly identical between the two modules.

4.4 Pressure Optimization

This section details the load bank testing and tuning of the system that lead to the reliable high power operation of the entire fuel cell system. Testing was conducted using the load bank to simulate full race conditions using the details described in Section 4.2 to simulate the race current profile. Control of the cathode pressure was critical to attaining peak performance. In addition, a few modifications were made to the anode supply system to allow peak performance, while maintaining proper cross pressure.
4.4.1 Cathode Pressure Tuning

As detailed in Chapter 2.1, fuel cells will generally attain their peak power when operating at the highest possible pressure. However, due to sharp dropouts in current draw with a vehicle transmission shift, the cathode gas system is exposed to sharp transient conditions. When the oxygen flowing through the cathode is being consumed at a high rate, less oxygen exits through the back pressure valve. When the current draw is temporarily removed, all unconsumed oxygen is forced through the back pressure valve, which raises the back pressure, and correspondingly the upstream pressure. In addition while running the fuel cell for long durations, the pressure drop of the cathode slowly increases, leading to a higher inlet manifold pressure at the end of the test compared to the beginning of the test.

Figure 4.24 shows the pressure dynamics of the cathode during a typical test run. The top plot of Fig. 4.24 shows the pressure drop across the cathode. This is the outlet pressure of the stack subtracted from the inlet pressure. The second
Figure 4.24: Cathode Pressure Dynamics during a Run.

The plot in the figure shows the upstream operating pressure of the cathode. The sharp spikes are the result of each shift, when the composition of the exit gases changes drastically.

A unique method to limit this pressure was discovered through the PRV system. The PRV’s were originally installed to prevent emergency overpressure situations, but the idea was proposed to use the PRV’s to limit peak pressures on each shift. The PRV’s were tuned to a setting just above the highest expected operating pressure that would occur near the end of the run. As the operating pressure rose, the PRV’s would be used on each shift to limit the peak cathode pressure. In this method
the PRV's acted similar to a blow-off valve for a turbocharged vehicle, and vented excess flow on each shift.

Figure 4.25: Peak Cathode Pressure is able to be limited by the PRV on each shift.

Figure 4.25 shows the result of the PRV when properly tuned to the cathode. The PRV is capable of controlling the peak pressure limits of the stack during shift sequences, while allowing the cathode to operate at a higher pressure between shifts. In addition, it was found through simple modeling that the pressure spikes are also reduced if more back pressure valves are used. Packaging allowed the room for an
additional back pressure valve to be added to the vehicle, leading a total of 3 back pressure valves for the shared exhaust volume.

### 4.4.2 Maintaining Proper Cross Pressure

It is critical to maintain a proper cross pressure on the membrane during fuel cell operation. The anode pressure should always be maintained above the cathode pressure. This is because the anode system is a closed system which recirculates the unused fuel, while the cathode is a flow through system that contains oxidant. The membrane is never quite a perfect seal, and small amounts of the gases will inevitably flow from the high pressure side to the lower pressure side. In this respect, if the cathode oxidant gases were to cross over to the anode side, where they were contained and recirculated, it may be possible to build up a combustible mixture of hydrogen and oxygen on the anode side. If there were a problem at the membrane, a hot spot could be developed that could ignite this mixture. In addition to the combustibility of the mixture, maintaining anode positive pressure also aids in keeping the concentration of hydrogen as high as possible at the anode, and reduces the needed number of purge cycles for the anode loop.

While the cross pressure should always favor the anode side, it also has to be controlled to a reasonable limit. Ideally the cross pressure could just be set very high to eliminate any worry, but this can cause a few problems. The largest problem is that the membrane is not able to handle too high of a pressure. The membrane is simply a thin film of polymer, and with enough pressure it is possible that it could rupture. This would result in a massive leakage of hydrogen to the cathode and possibly result in a combustible mixture of gases exiting the cathode, and therefore
exiting the vehicle. Another concern for limiting the cross pressure is that the membrane could simply deform toward the cathode side, which would increase the flow resistance to the cathode gases. The third concern is that the peak pressure is to be controlled altogether. Therefore the pressure of both the cathode and anode should be maximized, right to the design limit. If the cross pressure is very high, and the anode is set to the operational limit, that will limit how high the cathode pressure can be, and therefore lower performance.

The control of the cross pressure is further complicated by the flow design of the stack. The Ballard stacks are set up in a counter flow layout. Most modern stack designs use this configuration. This means the anode gas enters on one side of the flow channel, and cathode gases enter at the opposite. Due to pressure losses down the length of the channel, there is a much larger pressure difference on the side that is the anode inlet and cathode exit. This is visually represented in Fig. 4.26 which shows a graphical representation of the flow and pressure losses. On the right side of the figure it shows that the delta pressure across the membrane is much higher than it is on the left side. If the cross pressure regulator were poorly adjusted, it would be possible for the anode pressure to fall below the cathode pressure on the left side of the figure. Thus a delicate balance is required to always maintain positive cross pressure, without exceeding the cross pressure limitation of about 700 mBar.

4.4.3 Anode Pressure Tuning

While much effort was put into controlling the cathode pressure, the previous section indicated it is not actually the limiting pressure in the fuel cell. The real pressure limitation is on the anode side. The Ballard hydrogen delivery system
uses a pressure reference regulator that maintains the anode pressure above the cathode pressure. So the total stack pressure limitation comes from the anode pressure. The anode pressure spikes on each shift because it is referencing the cathode pressure. However the anode pressure actually faces an even higher change between its operating pressure and its pressure spike on each shift.

This higher pressure spike is due to the regulator droop of the pressure reference regulator in the anode system. This is best shown in Fig. 4.27. The figure points out the regions such as start up and shutdown where little to no current is being drawn. During these times the delta pressure regulator is able to achieve a static pressure setting. In the center is the region of high current draw, which is only interrupted momentarily by shifts. When the regulator is supplying hydrogen gas to match the flow rate required for high current operation, it experiences heavy flow losses, and cannot maintain the same pressure difference as it can in its steady state.
pressure setting. Then when a shift occurs, hydrogen consumption is momentarily stopped because current draw reaches zero. Thus on each shift the regulator can then reach its static pressure reference setting. With a simultaneous increase in cathode pressure, this leads to an even higher anode pressure.

![Figure 4.27: Hydrogen Pressure minus Oxygen Pressure to demonstrate the hydrogen regulator pressure droop.](image)

Figure 4.28 shows the anode and cathode pressures during a shifting condition. Since the cathode gas continues to flow through the mass flow controller, the cathode still shows a pressure drop. It also has an increased overall pressure because of the increase in back pressure due to the extra oxygen being forced through the back pressure valve. Since the hydrogen is not being consumed, it does not display a pressure drop, however the delta pressure gets even higher because the pressure droop of its regulator is no longer present.

A similar solution to the cathode PRV tuning was found to help limit the hydrogen pressure spikes, while maintaining the highest possible hydrogen pressure.
Figure 4.28: A visualization of the cross pressures during a shift.

during normal operation. The Ballard hydrogen supply system already contained a PRV valve. The valve was located downstream of the stack, attached to the same line as the purge valve. The valve is really installed as a marginal safety measure for the stack, as the single valve wouldn’t be capable of releasing the full flow rate the hydrogen regulator could provide. In addition, the valve was set fairly close to the design limit, at about 3 Bar. The particular valve is not as easily tunable as the Fisher 289 valves for the cathode. In addition, it is not a piloted valve, it simply cracks at a setting, but the flow resistance increase as the flow rate increases.

The anode PRV valve did have a variety of springs that were available from its manufacturer. By ordering the spring set that is just below the original one, the cracking pressure of the valve was able to be manually adjusted to be just above the steady state operating pressure of the Anode system under full load. In addition, since the highest pressure on the anode side was up stream of the stack, a second
anode PRV was added to the upstream portion of the anode loop, providing two separate PRV’s for the anode loop.
Figure 4.29: The result of properly tuning and installing a 2nd PRV for the anode system
Figure 4.29 shows the results of the tuning done to the anode system. The three modifications that were made to the anode system were the installation of the second PRV on the upstream side, properly tuning both the downstream and new upstream PRV, and finally the proper adjustment of the cross pressure regulator. These three adjustments combined resulted in the ability to run the anode at a higher steady state operating pressure under high load, while reducing and controlling the peak pressure obtained during a shift. The adjustments on the anode side were particularly small and sensitive relative to the adjustments for the cathode. The reason for this is likely the significantly smaller volumes in the anode side.

4.4.4 Conclusion of Pressure Tuning

At the conclusion of the pressure testing, adjustments, and design changes that were made to the BB2 fuel cell system, the BB2 fuel cell system was sealed up and shipped to Bonneville for the record setting runs. During the two week period, the fuel cell system performed flawlessly, and zero adjustments were made to any of the pressure regulators, PRV’s, or BPV’s. During the race event, the vehicle never failed due to any fault of the fuel cell system. As power demand was increased further and further through adjustment to the motor’s inverter, the fuel cell supply system was always able to provide the requested power, all while providing clean reliable cell voltages.

The robustness of the solution is best exemplified by showing the current draw and power generated during the record run of the race vehicle as shown in Fig. 4.31. As the figure shows, each fuel cell module easily exceeded 400 amps for a majority of the run. In addition, the fuel cell power was well over 500 kW for most of the run,
Figure 4.30: The total summation of pressure control and pressure relief devices used in the BB2 gas supply system and peaked near 540 kW. This is quite impressive for a system that was originally designed for a peak power of 250 kW. While no official record for this exists, this is most likely the most powerful automotive fuel cell system ever created, and will likely remain that way for quite some time.

4.5 Water Measurement Testing

Model development showed that the water outlet flow rate was likely a very important aspect to properly modeling the pressure dynamics of the BB2 system.
The problem was that during all previous BB2 testing, both with the load bank, and on the track, there was no way to record and measure the outlet flow rate of liquid water. In fact this is a common problem in fuel cell testing. There are not really any instruments that are capable of measuring flow rates of both liquid and gas phases of flow.

Relative humidity sensors are only capable of measuring flows that are below saturation conditions. The only way to measure the outlet water flow rate would be to inject a known amount of dry gas into the outlet flow stream, to bring the mixed
flow below saturation conditions, then measure the gas flow rate and humidity of the resultant stream. While this may be possible for a single cell test, or a very low power stack, the flow rate of gas and test setup to do this type of test for the BB2 would be nearly impossible, and certainly unpractical.

### 4.5.1 Water Test Setup

The advantage the BB2 has for measurement of the water outlet flow rate is the massive amount of water that is generated compared to a lower power fuel cell system. Previous observations of the testing indicated that significant and likely measurable amounts of water could be produced during a test run. Based on this observation a test was setup to capture the water and record its weight in real time. Figure 4.32 shows the test setup.

![Figure 4.32: The Water Measurement Test Setup](image)

The exhaust from both sides of the vehicle (two exhaust ports on the right, and one on the left) was routed through long tubes, and pointed directly at a large basin. Under the basin a digital scale was placed.
The digital scale is an Ohaus explorer pro scale with a range of 32000 grams, and a resolution of 0.1g, making it an extremely sensitive scale relative to the desired measurement. The scale is equipped with an RS232 communications port, and is capable of printing out the scale reading over serial communication. A matlab script was setup to continuously request scale print outs of the weight, and the weight and time were written to a text file. The Baud rate of the serial communication of the scale was set at its maximum of 9600. With this slow baud rate, the scale measurements could be taken roughly 5-6 times per second.

Several other methods of water collection were discussed. Ideas such as diverting the air into a chamber with a small liquid drain, or flowing the air at a plate, and letting the liquid drip down the plate to a collection tub were proposed. However, the practicality of running these test were one limitation. Also, if the water were collected or diverted into a secondary object, there would be a longer delay for the water to be measured. For these reasons the simple method discussed above was used.

4.5.2 Raw Test Results

Five test runs were conducted, with only three providing meaningful data, and only two of the runs being long enough to be analyzed with the model. The first test resulted in a fault with the scale recording communication. During the second test run, the data was cut short because of a fuel cell fault. This run however provided a useful data point due to a sharp cutoff in the gas flow rate that could be read by the scale. The third run was an full duration run, but the operating pressure was
not set as high as it had been in Bonneville to provide the required peak current and power without crashing the cells.

<table>
<thead>
<tr>
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</tr>
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<tbody>
<tr>
<td>1</td>
<td>Scale Recording error</td>
</tr>
<tr>
<td>2</td>
<td>Fuel Cell Fault with Sharp Shutdown</td>
</tr>
<tr>
<td>3</td>
<td>Operating Pressures not high enough for sustained high current performance</td>
</tr>
<tr>
<td>4</td>
<td>Shifting, with PRV’s Disabled</td>
</tr>
<tr>
<td>5</td>
<td>Long Steady State Run</td>
</tr>
</tbody>
</table>

Table 4.3: Water Measurement Tests.

The final two runs provided two separate good sets of data that can be used for model validation. Test 4 was a test run where three simulated shifts were commanded during the test. Test 5 was simply a long duration test run with a constant current draw at nearly identical levels to the vehicle race data from Bonneville.

Figure 4.33 shows the scale recorded weight vs time for the 4th scale test. Also on the plot are the recorded inlet flow rates of heliox from the mass flow controllers. As the plot shows, despite a constant command to the mass flow controllers during peak power, they do not provide a perfectly constant air flow rate.

The scale reading shows five peaks that require some explanation, and will require some post processing to compensate for. Its quite obvious that when recording water being dumped into a tub, there should not be times when the weight goes down. Unfortunately, due to the practicality of setting up the test, the scale reading is being influenced by the outlet flow rate of gases.
The first peak seen is due to the start up of the system as gas flow rate is ramped up. The spring action of the BPVs has always made this an unstable region for the gas exit flow. The system is a bit unsteady until enough air flow is exiting for the BPVs to act in a smooth controlled manner.

The middle 3 peaks occur when a simulated shift is commanded with the load bank. During these shifts, a significant increase in flow rate of exiting gas occurs because none of the oxygen is being consumed, leading to more gas being forced out the exhaust and directed toward the scale.

The final peak is when the system was shut off quickly, and the gas flow stopped altogether. The scale then records the total amount of water that has been accumulated during the run.
4.5.3 Correcting the Weight Measurements

It is clear that the exiting air flow rate is affecting the real time weight measurement of the scale. In order to correct for this, the simple idea of aerodynamic drag will be applied to correct the scale reading. The standard equation for aerodynamic drag is shown below. All the terms except $V^2$ are essentially constants the depend on the particular flow being considered.

$$F_{aero} = \frac{1}{2} \rho C_d A V^2$$

(4.1)

For the scale reading to be corrected properly, two things need to determined, the value of the constants, and the real time value for $V^2$. As Fig. 4.33 showed, scale is directly influenced by the outlet flow rate of the gases, not the inlet flow rate of gases. Fortunately the failed test number 2 actually provides the needed data to determine these parameters.

During the execution of test 2, a component in Module B was not operating properly, and the Ballard Controller commanded a hard shutdown of the stack. This simultaneously opened the electrical contacts and shut off gas flow under full flow conditions. Figure 4.34 shows the data during this run. At approximately 55 seconds the air flow is steady, along with the current consumption. Suddenly both are shut off, and the scale instantly drops .32 kg in reading. So this test provides the aero force applied to the scale, but the exiting flow rate in real time needs to be determined as well.

The control oriented model detailed in Chapter 3 is later shown to be incapable of predicting the complete pressure dynamics. However, it is perfectly capable of calculating gas exiting flow rates. The model uses the known air inlet flow rates,
Figure 4.34: The recorded data during a hard shutoff of air flow and the current draw of the stack to calculate gas consumption. Therefore the model is exactly calculating the exiting gas flow rate. When the model is applied during the failed test run 2, the exiting flow rate during the shutdown can be calculated, and used to find the constants for correction. Just before the shutdown of the test the exit flow rate is .0385 kg/s.

This data is used in the simulator to provide a correction force that is applied to the scale due to the gas velocity. The following two plots show the corrected scale reading as applied to Tests 4 and 5.

Figures 4.35 and 4.36 show the original scale reading, along with the exiting gas flow rate. The exit gas flow rate is used to calculate the corrected scale reading. This method is not exactly perfect, especially at the beginning of the test. As mentioned before, the start up often has fairly unstable flow due to the lower flow rates. The
Figure 4.35: The corrected scale reading for Test 4

Figure 4.36: The corrected scale reading for Test 5
method does help clean up the readings a bit. It lessens the peak reading during the shifts, and provides that the final scale reading of the corrected plot matches up with the final scale reading of the raw data after gas flow has stopped.

4.6 Pressure Drop Testing

One portion of the model that needed some data analysis was the evaluation of the pressure drop without the confounding variable of current draw, or excess water droplet removal. To accomplish this testing, various air flow commands were given to the mass flow controllers, and the air flow rate and pressure drop were recorded for each module over a series of two tests.

In the first test, lower flows were commanded and most of the water that remained in the system was expelled. Various air commands were given to provide a range of flow rates. At full current request in race conditions, the mass flow controllers are given a flow command of 56.3%, which was commanded in both tests. Unfortunately a limited availability of the test gases prevented further testing. Figure 4.37 shows a sample of the air flow command and air flow rates for the second test.

Unfortunately, when running manual tests like this, the communication link between the computer that gives the commands and the Ballard controller can experience some delay. The problem is that there are two mass flow controllers which need to be given override signals simultaneously. To do this, two separate computers are setup, and the new flow rate command is entered into each computer simultaneously. However as Fig. 4.37 shows, the input commands do not hit the
controller at the same time. This leads to limited samples of data that can be gathered when the air flow rates are near the same amount.

4.6.1 Pressure Drop Results

The results of the pressure drop testing are shown in Fig 4.38. The results show a fairly linear pressure drop compared to the inlet flow rate. They also show that the pressure drop near maximum flow rate will be around 0.18 Bar. The data is a bit noisy, but this is due to the inability of the mass flow controllers to provide a perfectly matched flow rate, as well as the method of pressure drop measurement. The pressure drop is measured by subtracting the pressure of two separate pressure sensors. While a true ∆P sensor may provide cleaner results, one was not available for use in the this pressure range.
4.6.2 Initial Water Conditions

An unexpected side benefit of running the pressure drop testing was that the initial water conditions of the stack were obtained. The testing was run with the humidifier turned off, and run until liquid water was no longer exiting the stack. During the runs the collection tub was placed under the exhaust tubes, and the total weight of water that exited was recorded. The weight was .74 kg. This represents the liquid water that is essentially left in the stack between runs. Every time the fuel cell system is run and then stopped, this would be the amount of water that would be in the system before the start of the next run. This amount of water will be used to provide the initial conditions of liquid water in the stack for the evaluation of the models developed.


4.7 Conclusions

This chapter provided the details of the experimental methods used for the BB2. First, a robust PRV system was developed to prevent the cathode pressure from exceeding the limitations of the stack. A fan-cooled resistor load bank was built by the team, and was used for system testing, including the simulation of transient conditions that result from vehicle transmission shifts. The load bank was then used to help test, tune, and optimize the settings for the cathode operating pressure. In addition, careful adjustments were made to the anode side to optimize its pressure performance, while minimizing pressure spikes during shifts, and keeping the cross pressure between the cathode and anode within limits.

Throughout the load bank testing, an imbalance between the two FCMs was discovered. Details of its discovery, and correction were provided. After the imbalance was corrected, the FCM currents were equalized during testing. After all the testing, tuning, repairs, and system changes, the fuel cell system became a robust power plant that powered the BB2 to its international speed records.

Finally, for the purposes of model validation, some additions test were run to measure liquid water outflow from the stacks. These measurements required a correction to be applied to the scale reading due to the outflow of gases which was measured by the scale.
CHAPTER 5

Modeling Results

This chapter presents the results of the modeling work that was detailed in Chapter 3. The chapter begins by presenting the results of the simplest model applied, the control oriented model based on the work of [60], and discusses some of its short comings and areas needed for improvement. Next, the results of a simplified model with two-phase flow considerations are shown with some improvement when the water outlet flows are considered. This shows that the water outlet flow rate is one of the critical aspects important to capturing the dynamics of the system.

Next the results of the laminar flow model are shown. Some discussion on the number of discretizations, and the pressure drop prediction of the model are discussed. The results are shown first with a single upstream stack resistance, and followed by two separate models with different methods of capturing the two-phase resistance downstream of the cathode.

All results are typically presented with two separate sets of test data. The first data set is from a load bank test with a relatively constant steady state current draw. The second set is from a load bank test where vehicle shifts were simulated by using sharp cut-offs in the current draw.
For most results, three parameters will be presented, the inlet manifold pressure from module A, the exhaust manifold pressure, and the pressure drop (which is simply the difference between the two). Where necessary additional plots will be provided. Module A inlet manifold pressure data is only presented here, but the models perform equally for Module B.

A section on model calibration is provided. First data are presented with a poorly calibrated model. Then, one at a time each parameter is adjusted and the new results shown and discussed.

Once the final model has been presented and calibrated to match the test stand data, its performance will be judged against data from the BB2 race data, and discrepancies discussed. Recommendations on modifications to the model and areas of future work will be discussed.

Table 5.1 summarizes the models whose results are presented in this chapter, and their various components. The table also assigns a model number to help the reader keep track of the model being evaluated.
<table>
<thead>
<tr>
<th>Model Number</th>
<th>Description</th>
<th>Resistance Upstream of Stack</th>
<th>Stack Water Flow Model</th>
<th>Resistance Downstream of Stack</th>
<th>Back Pressure Valve Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Control Oriented Model Adapted from Pukrushpan et al</td>
<td>None Used</td>
<td>Liquid water flow not considered.</td>
<td>Linear resistance for gaseous phase only</td>
<td>Single Phase Model</td>
</tr>
<tr>
<td>2</td>
<td>Control Oriented Model with Two Phase Flow Correction</td>
<td>None Used</td>
<td>Liquid water outlet flow proportional to the mass of liquid water in the cathode volume</td>
<td>Linear resistance with outlet flow rate proportional to mass of water in the cathode</td>
<td>Two-Phase Model based on Area Reduction</td>
</tr>
<tr>
<td>3</td>
<td>Distributed cathode model for water outflow prediction</td>
<td>Linear resistance, considers inlet gas only</td>
<td>Distributed laminar flow model</td>
<td>None Used</td>
<td>Two-Phase Model based on Area Reduction</td>
</tr>
<tr>
<td>4</td>
<td>Distributed model, upstream and simple downstream resistance model</td>
<td>Linear resistance, considers inlet gas only</td>
<td>Distributed laminar flow model</td>
<td>Linear resistance with outlet flow rate proportional to the mass of water in the cathode</td>
<td>Two-Phase Model based on Area Reduction</td>
</tr>
<tr>
<td>5</td>
<td>Distributed model, upstream and two phase eqn downstream</td>
<td>Linear resistance, considers inlet gas only</td>
<td>Distributed laminar flow model</td>
<td>Resistance based on published two phase flow through a restriction</td>
<td>Two-Phase Model based on Area Reduction</td>
</tr>
</tbody>
</table>

Table 5.1: Attributes of the models whose results are evaluated in this chapter.
5.0.1 Modeling Inputs

The data recorded from the BB2 testing can be used to test the model of the BB2 cathode system. The inputs to the overall system model are the air flow rates through the mass flow controllers, the stack operating current, and stack temperature. All these parameters were recorded through the testing, and can be fed to the model.

A note should be made about the input conditions. For the most part, under a large portion of the data set, the Heliox inlet flow rate is set and held at a steady constant value to provide the required flow. There is some variation in the flow rate due to poor performance of the mass flow controllers, but the command remains the same. What may change throughout the run is the operating current.

For the comparison of the performance of the 5 models evaluated in this chapter, two separate sets of test data will be used. In the first test a relatively constant load was set and held as long as possible. The second test was conducted with three simulated shifting sequences. The input currents for the constant current and shifting tests are shown below in Fig. 5.1. Figure 5.1(a) shows the current drawn during the constant load test. The current profile shown in Fig. 5.1(b) shows three distinct drops in the current draw that occur with each simulated shift, when no power is consumed.
Figure 5.1: The Current Profiles from two sets of static tests used to evaluate the model performance.

This data was recorded during static testing after the BB2 had set its record runs. For the testing the PRV’s on the cathode were disabled to minimize the variables in the model calibration.

5.0.2 Modeling Outputs and Metrics

Pressure sensors record upstream and down stream pressure, and are compared to the results of the model. Three separate parameters are of concern: the inlet manifold pressure, the back pressure (or exhaust manifold pressure), and the pressure drop across the cathode. For each model evaluated, these three results will be presented.

The results of the model will be compared to the results of the simulator. To find an objective measure of the models ability to match the data, a set of metrics is presented, and will be used in all cases to evaluate the relative performance of the models.
The model performs poorly during startup and shutdown periods of the system. During start up this is due to the linearized stack resistance, and the unsteady performance of the back-pressure valves during very low flow conditions when they tend to surge. During shutdown, the linearized stack resistance again causes errors which are coupled with the poor performance of the mass flow controllers during shutdown when the upstream pressure is falling due to the depleted pressure supply from the tanks. For these reasons, a time window during steady operation will be considered for each metric. For the steady current test, this is from 16 seconds to 91 seconds. For the shifting test this is from 12 to 77 seconds.

**Mean Absolute Error**

The first metric is one which considers the overall error between the model and the data, and will be called the mean absolute error. To evaluate the mean absolute error, the absolute value of the error between the model and the data will be integrated, and divided by the time interval. This is reflected in the equation below.

\[
\text{Mean Absolute Error} = \frac{\int_{t_1}^{t_2} |P_{\text{data}}(t) - P_{\text{model}}(t)|}{t_2 - t_1} \tag{5.1}
\]

**Offset Error**

The next metric evaluates the error, but eliminates any steady offsets that may be present. To do this, the average value over the period of time is subtracted from the pressure values at any given instant in time. This metric would help in evaluating the model performance if there was a steady pressure offset present, but the slopes of the data were well matched. The equation for the calculation of this
metric is below.

\[
\text{Offset Error} = \int_{t_1}^{t_2} \left| \frac{P_{\text{model}}(t) - \text{avg}(P_{\text{model}})_{t_1}^{t_2}}{t_2 - t_1} - \frac{P_{\text{data}}(t) - \text{avg}(P_{\text{data}})_{t_1}^{t_2}}{t_2 - t_1} \right| \tag{5.2}
\]

**Pressure Rise**

In all the pressure results evaluated (inlet pressure, outlet pressure, pressure drop), there is a relatively low frequency rise between the start and end of the run. To capture this rise, a fairly simple metric is used. This metric simply takes the pressure difference between the start and stop time of the data, and compares it to what is seen in the data. The start and stop times for this metric were chosen based upon the relatively highest and lowest points in the data under the steady conditions. For the constant test, the start and end times used are 25 and 80 seconds. For the shifting test the times are 13 and 75 seconds.

\[
\text{Pressure Rise Error} = [P_{\text{model}}(t_2) - P_{\text{model}}(t_1)] - [P_{\text{data}}(t_2) - P_{\text{data}}(t_1)] \tag{5.3}
\]

**Pressure Spike Prediction**

The final metric is used only for the shifting tests that were conducted. During shifts, there are pressure spikes in the inlet manifold and exhaust manifold pressures that need to be modeled. Also, the pressure drop sometimes shows spikes in the model that are not seen in the data.

To provide a way to evaluate the model’s ability to capture these spikes appropriately, a pressure spike prediction metric is created for each shift. To do this, a 5 second window is defined around each shift, and the maximum and minimum pressures within this window are found. Then the error for a single shift is the difference between the maximum and minimum pressure of the data, subtracted from
the difference between the maximum and minimum pressure of the model. This is reflected in the equation below.

\[ \text{Err}_\text{N} = (P_{\text{max}} - P_{\text{min}})_\text{data} - (P_{\text{max}} - P_{\text{min}})_\text{model} \]  

(5.4)

The final value of the metric is the average of the error for all 3 of the shifts that were conducted.

\[ \text{Shift Error} = \text{avg}(\text{Err}_1, \text{Err}_2, \text{Err}_3) \]  

(5.5)

5.1 Control Oriented Model (Model 1)

The first model evaluated is Model 1, which is the adaptation of the model from [60] to match the parameters of the BB2. The pressure dynamics are explored first. Then some problems with the model are identified. These problems lead to the development of Models 2-5 that are evaluated later in this chapter.

5.1.1 Pressure Results of Model 1

The following three sections explore the results of the pressure dynamics for Model 1. The results are presented for the inlet manifold pressure, the outlet manifold pressure, and the cathode pressure drop for both a constant current test and a test with simulated shifts. Table 5.2 shows the settings of relevant tunable parameters used in the model to get the results presented.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
<td>31</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{\text{DS}}$</td>
<td>$1.8e^{-6}$</td>
<td>$kg/(Pa-s)$</td>
</tr>
</tbody>
</table>

Table 5.2: Calibration Parameters Model 1
**Inlet Manifold Pressure of Model 1**

The results of feeding the recorded inputs to the model are shown in Fig. 5.2, which compares the recorded cathode pressure to the model. Figure 5.2(b) shows three separate pressure spikes. These occur when a shift is simulated. The pressure spikes are a result of the drastic changes that occur to the gas flow rate when oxygen is being consumed at a high rate, and is then suddenly re-introduced into the flow stream and forced through the exhaust.

![Graphs showing inlet manifold pressure results for Model 1](image)

(a) Results With Constant Load  
(b) Results With Shifting

**Figure 5.2: Model 1 Inlet Manifold Pressure Results**

<table>
<thead>
<tr>
<th></th>
<th>Constant Load</th>
<th></th>
<th>Shifting</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
<td>Press. Rise Err</td>
<td>Mean Abs Err</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.119</td>
<td>0.068</td>
<td>0.152</td>
<td>0.112</td>
</tr>
</tbody>
</table>

**Table 5.3: Inlet Manifold Pressure Metrics for Model 1**
Fig. 5.2(b) shows the pressure spikes that occur with each gear shift. The modeled pressure shows pressure spikes that correspond to each shift, but do not match the peak magnitude of the recorded data. Figure 5.2(a) shows that the steady state operating pressure increases as the run progresses, which is not captured by the model. Table 5.3 shows the error metrics calculated for the inlet manifold pressure, which will be compared to the metrics of other models later in the chapter.

**Exhaust Manifold Pressure of Model 1**

Fig. 5.3 shows the exhaust manifold pressure compared to the model. From the figure several major discrepancies are observed. Figure 5.3(b) shows that the pressure spike on shifts is nearly non-existent with the modeled back-pressure valve. Figure 5.3(a) shows that there is also an increase in the steady state operating pressure seen in the data as the run progresses that is not captured by the model.

(a) Results With Constant Load  
(b) Results With Shifting

Figure 5.3: Model 1 Exhaust Manifold Pressure Results
Table 5.4: Exhaust Manifold Pressure Metrics for Model 1

Table 5.4 shows the error metrics calculated for the exhaust manifold pressure, which will be compared to the metrics of other models later in the chapter.

**Cathode Pressure Drop of Model 1**

To gain a better understanding of the pressure dynamics, the pressure drop is examined. The pressure drop is simply the exhaust manifold pressure subtracted from the inlet manifold pressure, but it provides another method to understand what is physically occurring, and to understand the problems with the model.

![Graphs of pressure drop results](image-url)

(a) Results With Constant Load  
(b) Results With Shifting

Figure 5.4: Model 1 Pressure Drop Results
<table>
<thead>
<tr>
<th>Units</th>
<th>Constant Load</th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
</tr>
<tr>
<td></td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.045</td>
<td>0.029</td>
</tr>
</tbody>
</table>

Table 5.5: Pressure Drop Metrics for Model 1

Figure 5.4(a) shows that the linearized pressure drop equation generally captures the general magnitude of the pressure drop during sustained operation, but that the pressure drop slowly increases during the run, which is not captured by the model. Figure 5.4(b) however, shows that during the transients that occur on each shift, the modeled pressure drop reaches a much higher spike than what is seen with the data. Table 5.5 shows the error metrics calculated for the inlet manifold pressure, which will be compared to the metrics of other models later in the chapter.

### 5.1.2 Problems with Model 1

Several fundamental problems have been found with the assumptions and model linearizations based on the model from [60] when it is adapted to the BB2 system. One assumption of the model is that the mass of the liquid water is accounted for, but it is assumed to not affect the pressure drop characteristics of the cell, assumed not to exit the cathode volume, and assumed to not obstruct the flow or reactants through the gas channel. In an actual fuel cell system, none of these assumptions are true. The liquid water effects the pressure drop because it obstructs the flow of reactants, and a significant amount of the liquid water exits the stack.

The assumptions of ignoring liquid water may very well be reasonable when dealing with lower power fuel cell systems, or systems operating at lower current
density, or for single cell tests. However, consideration of the liquid water becomes critical for the high power system of the BB2, where a large amount of current is being generated by a very large fuel cell stack. Static testing shows that significant amounts of liquid water droplets exit the fuel cell system, as can be qualitatively seen in Fig. 5.5.

![Figure 5.5: Water spray during a system test.](image)

The mass of the liquid water that accumulates in the cathode is computed by the model, which does not allow the liquid water to leave the cathode volume. During a full length simulated run, nearly 3.5 kgs of water could be generated and accumulated in each cathode volume, as shown in Fig. 5.6.

Since the exit flow of the liquid water is not accounted for in the model in [60], major problems occur in the implementation for the BB2. The first problem is that during a shift, a large spike in the pressure drop is seen. In fact, during high current operation, the model takes into account the consumption of the oxygen, and replaces
it with water vapor, which has nearly the same mass. However since the flow is fully saturated, the water vapor is essentially all turned into water droplets. During the high current operation, a large amount of water droplets will flow through the cathode, but since there is no way to account for their mass flow rate, they do not affect the pressure drop in any appreciable way.

When a shift occurs, suddenly oxygen is no longer being consumed, and is forced to flow through the linear stack resistance model. This extra mass flow rate requires a higher pressure drop to pass the resistance, leading to the spike in the pressure drop with each shift that is seen in the model.

Another observed problem is that the back pressure valve model is not as restrictive in the model as it is in the test data. In addition, as the run progresses, the back pressure does not show an appreciable increase, and therefore the cathode
pressure does not show the pressure increase that is seen in the data. This can also be explained because the water outlet flow is ignored in the model. The water droplets that become entrained in the exhaust flow lead to significantly more mass being pushed through the back pressure valve than is accounted for in this model.

The gradual rise in the operating pressure seen in the data but not reflected by the model is explained with a hypothesis. As the fuel cell system begins running, water is slowly building up inside the system. Early in the run, the exiting water flow rate is a bit lower than it is near the end. As the run progresses, the water builds up and the system begins to reach a steady state condition, and more and more liquid water is forced to flow out through the exhaust. This leads to an even higher mass flow rate through the back pressure valve near the end of the run, explaining the gradual rise in the pressure.

5.1.3 Model 1 Conclusions

In summary, there are 4 discrepancies between the model and test data that were seen in Figs. 5.2-5.4.

1. There is a gradual increase in the operating pressure as a test run progresses that is not captured by the model.

2. The data shows a spike in back pressure that occurs during each shift, but is not captured by the model.

3. The data shows a slow increase in the pressure drop as the run progresses that the model does not capture.
4. The modeled pressure drop show large spikes with each shift that are not seen in the data.

5.2 Control Oriented Model with Simple Two Phase Consideration (Model 2)

The next model evaluated takes the Control Oriented Model (Model 1) and adds some simplified calculations to deal with two phase flow considerations. The stack resistance is changed to be proportional to the total flow of liquid and gas. The outlet flow of the water is set to be proportional to the amount of liquid water in the cathode relative to a tunable maximum amount of water allowed. The exhaust manifold model is changed to track the inlet and outlet flows of liquid water. The back pressure valve model is recalculated to change the valve’s effective $C_dA$ proportional to the mass of water in the exhaust manifold. The outlet flow rate of the liquid water is always proportional to its instantaneous mass fraction relative to the gas.

5.2.1 Pressure Results of Model 2

The following three sections explore the results of the pressure dynamics for Model 2. The results are presented for the inlet manifold pressure, the outlet manifold pressure, and the cathode pressure drop for both a constant current test and a test with simulated shifts. Table 5.6 shows the relevant parameters used in the simulation of Model 2.

Inlet Manifold Pressure of Model 2

Figure 5.7 shows the results for the inlet manifold pressure when Model 2 is evaluated. Figure 5.7(a) shows that the model begins to do a much better job capturing
Table 5.6: Calibration Parameters Model 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{preset}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.02</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$kgs_{max}$</td>
<td>1.2</td>
<td>kg</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>$3.7 \times 10^{-6}$</td>
<td>kg/(Pa - s)</td>
</tr>
</tbody>
</table>

the steady slow rise in operation pressure as the run progresses. Unfortunately Fig. 5.7(b) shows that the pressure spikes are significantly higher for each shift than they were in Model 1. This is explained because the single downstream resistance is now accounting for the mass of liquid water and the gas, and on each shift some amount of water is also traveling through this downstream resistance.

Figure 5.7: Model 2 Inlet Manifold Pressure Results

(a) Results With Constant Load  
(b) Results With Shifting
<table>
<thead>
<tr>
<th>Units</th>
<th>Constant Load</th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.119</td>
<td>0.068</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.041</td>
<td>0.039</td>
</tr>
</tbody>
</table>

Table 5.7: Inlet Manifold Pressure Metrics for Models 1-2

Table 5.7 Shows the inlet manifold metrics compared between Models 1 and 2. The table confirms what is seen in Fig. 5.7. The error metrics are improved in almost all cases with Model 2, while the pressure spike error is greater in Model 2.

**Exhaust Manifold Pressure of Model 2**

Figure 5.8 shows the results of the exhaust manifold pressure when Model 2 is applied. The results seen in Fig. 5.8(a) show that the steady rise in the back pressure is captured by Model 2, unlike Model 1. Model 2 also shows spikes in the back pressure that were not seen in Model 1, as seen in Fig. 5.8(b). Unfortunately the magnitude of the pressure spikes exceeds what is seen in the test data.
(a) Results With Constant Load

(b) Results With Shifting

Figure 5.8: Model 2 Exhaust Manifold Pressure Results

<table>
<thead>
<tr>
<th></th>
<th>Constant Load</th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.075</td>
<td>0.044</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.026</td>
<td>0.025</td>
</tr>
</tbody>
</table>

Table 5.8: Exhaust Manifold Pressure Metrics for Models 1-2

Table 5.8 shows the metrics for the exhaust manifold for Models 1 and 2. Most of the error metrics show improvement from Model 1. Its interesting to note that the pressure spike error is worse for model 2 on the inlet manifold, but better for the exhaust manifold. This is because the exhaust manifold pressure in Model 1 showed no spikes at all. So despite the fact the spikes are too high in Model 2, the metric shows better spike error than Model 1.
Cathode Pressure Drop of Model 2

The results of the cathode pressure drop are shown in Fig. 5.9. During the steady current test seen in Fig 5.9(a), Model 2 does a better job of capturing the steady rise in pressure drop throughout the run. However, Fig. 5.9(b) shows that the pressure drop with each shift is still seen to spike very high with Model 2, which does not match the data very well at all.

![Figure 5.9: Model 2 Pressure Drop Results](image)

(a) Results With Constant Load          (b) Results With Shifting

<table>
<thead>
<tr>
<th></th>
<th>Constant Load</th>
<th></th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
<td>Press. Rise Err</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.045</td>
<td>0.029</td>
<td>0.069</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.019</td>
<td>0.019</td>
<td>0.031</td>
</tr>
</tbody>
</table>

Table 5.9: Pressure Drop Metrics for Models 1-2
Table 5.9 shows the metrics for the pressure drop performance of models 1 and 2. The metrics are generally reduced in all cases as model 2 matches the pressure drop much more closely than model 1.

5.2.2 Water Outflow Results of Model 2

Since Model 2 is the first model to consider the outlet flow rate of water, the simulated water outlet flow can be compared to the water test data discussed in Chapter 4. As mentioned in the testing section, the water was measured on a scale, and the data was a bit noisy, and had to be corrected to account for the gas flow that was affecting the scale reading. When this data is analyzed to look for a flow rate of the exiting water, it is simply too noisy to get a reasonable estimate of the water flow rate vs time. Instead, the total accumulation of water must be analyzed to compare the test data to the model. To do this a simple integrator block for the exiting flow rate is used in the simulator.

Figure 5.10: Model 2 Water Exit Results

(a) Results With Constant Load
(b) Results With Shifting

Figure 5.10: Model 2 Water Exit Results
Figure 5.10 compares the simulated water output between Model 2 and the test data. As the data shows, the simplified model for accounting for the water outlet flow rate used by Model 2 greatly overpredicts the water flow compared to the test data. This means a different method for simulating the water outlet flow rate should be considered.

5.2.3 Model 2 Conclusions

Model 2 shows a significant improvement over Model 1 in several areas. First, it is able to predict the low frequency rise in inlet manifold pressure, exhaust manifold pressure, and the pressure drop. Unfortunately, it also greatly overpredicts the pressure spikes in the exhaust manifold pressure and the inlet manifold pressure for each shift. In addition, the pressure drop spikes on each shift. The outlet water flow predicted by this simplified model also greatly overpredicts the experimental measurements.

The improvements seen in the performance of Model 2 are a result of the consideration of the effect of the outlet water flow on the back pressure and the cathode pressure drop. However, improvement needs to be made in the calculation of the pressure drop, as well as the rate at which water leaves the module.

5.3 Discretized Flow Model (Model 3)

This section discusses the results when Model 3 is evaluated. Model 3 replaces the cathode model with a distributed parameter model that is used to predict the outlet flow rate of water with the discretized laminar flow model developed in Chapter 3. Upstream of this model is a single linearized flow resistance that is similar to the resistance used in Model 1. Before the pressure results can be analyzed, some
other areas of the model should be analyzed. First a decision on the number of discretizations used in the analysis is discussed. Next, the performance of the model is evaluated by looking at the water height in the channel calculated by the model, as well as evaluating the pressure drop predicted by the model. Next the water outlet flow of the model is discussed to see if the tunable velocity-slip parameter $alpha$ should be used in the evaluation of the pressure results. Finally the inlet manifold pressure, exhaust manifold pressure, and pressure drop of the model are analyzed.

5.3.1 Number of Discretizations for Model 3

The discretized model that was developed leaves open the question of how many discretizations to use. The general answer is typically the more the better. However, for practical purposes, the limit of what is required to get reasonable accuracy with minimum computational time should be explored.

To evaluate these considerations, a set of simulations was run, and the number of discretizations was changed between 1 and 13. A number of discretizations above 13 began to take a long time to solve, but the results show it is unnecessary to explore any larger numbers of discretizations.
Figure 5.11: A comparison of the model output relative to the number of discretizations.

Figure 5.11 shows the results of the investigation. The plot shows the water outlet flow rate vs time for each of the various numbers of discretizations. The results show that increasing the number much above seven leads to fairly similar flow rate results for the water flow. For this reason the number of discretizations used for all the results presented will be seven discretizations.
5.3.2 Water Height and Pressure Drop of Model 3

To explore the performance of the discretized model, a few of the parameters of the model are investigated. First the height of the water film in each discretization is explored. When Model 1 is run with some test data, it indicates that if no water were to leave the system, and a full length Bonneville run were made, about 3.3 kg of water would remain in each module. Simple geometric calculations show that if no water were to exit the cathode, and it were equally dispersed along the cathode channels, this would result in a even film height of of .145mm in a 1mm channel. We expect the model would show less height than this, since water is allowed to exit. Figure 5.12 shows the real time calculated water film height vs time for each discretization.

Figure 5.12 shows the model is performing within reason. The height of water is well within the expected range. There is an increase in the water height with each subsequent discretization. This is to be expected, as the current distribution is assumed to be even which means the water is generated equally along the flow path, but is forced toward the exit of the cathode due to the gas flow.

The discretized model also relies on the pressure drop between each discretization to force the flow of the gases. However Section 3.6 showed the dry gas laminar flow pressure drop calculation and suggested the total pressure drop for a dry channel is quite small, especially compared to the pressure drop seen in the data. Therefor, the pressure drop between each discretization is expected to be even smaller. Figure 5.13 confirms this, showing that the pressure drop between each discretization is around .4 mbar, for a total of roughly 3 mbar. This agrees well with the dry gas calculations which predict the total pressure drop to be 3.7 mbar. However, the total
measured pressure drop of the entire system is around 200 mbar, several orders of magnitude higher than the laminar calculations can account for.

5.3.3 Water Outlet Flow of Model 3

The model is clearly not capable of explaining the total flow pressure drop seen in the data between the inlet manifold and the outlet manifold. However hopefully it is capable of explaining the water outlet flow rate, specifically how it varies as the fuel cell is ramped up to full current draw.
Figure 5.13: Pressure Drop with modified model.

Figure 5.14 shows the comparison of the weight measurement for the two test runs vs. the modeled water accumulation that would exit the systems.

As the test data shows, Model 3 does a much better job correlating with the experimental results than Model 2. There is a slow ramp up of water at the beginning of the run, and it slowly appears to reach a quasi steady state increase in weight toward the end of the run. This corresponds with a physical idea of what might occur. As the cell begins creating product water, it builds up initially, and eventually
reaches a steady state output where it is being forced out at the same rate it is generated.

While the model does an excellent job correlating with the data, a quick experimentation with the tunable $\alpha$ parameter is also investigated. The value of $\alpha$ creates a slip between the gas and water velocities in the laminar flow model. In the steady state current results seen in Fig. 5.14(a), the model very slightly out predicts the measured water output. Figure 5.15 compares the constant current draw test with a value of $\alpha = 1.0$ to a value of $\alpha = 0.1$.

The value of alpha appears to slightly alter the results for the better, but appears to under predict the output at the beginning of the run. Since the original value of $\alpha = 1.0$ appeared to do reasonably well for both the constant current and shifting case, it will be used in further presentation of the results. In addition, all further modeling presented in this chapter will use the same cathode flow model, so the
Figure 5.15: Comparison of water outlet flow plots with two different values of $\alpha$

water outlet flow plots will be the same, and do not need to be presented again for Models 4 and 5.

5.3.4 Pressure Results of Model 3

With the number of discretizations finalized at seven, and the value of $\alpha$ confirmed at 1.0, the following sections will detail the results of the pressure dynamics when simulations are run for Model 3. Results of inlet manifold pressure, exhaust manifold pressure, and cathode pressure drop are presented and discussed. Table 5.10 shows the relevant parameters used in the evaluation of Model 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.02</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$3.7e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
</tbody>
</table>

Table 5.10: Calibration Parameters Model 3
Inlet Manifold Pressure of Model 3

Figure 5.16: Model 3 Inlet Manifold Pressure Results

<table>
<thead>
<tr>
<th></th>
<th>Constant Load</th>
<th></th>
<th>Shifting</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Offset</td>
<td>Press.</td>
<td>Mean</td>
</tr>
<tr>
<td></td>
<td>Abs Err</td>
<td>Error</td>
<td>Rise</td>
<td>Abs Err</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.119</td>
<td>0.068</td>
<td>0.152</td>
<td>0.112</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.041</td>
<td>0.039</td>
<td>0.033</td>
<td>0.057</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.067</td>
<td>0.039</td>
<td>0.055</td>
<td>0.074</td>
</tr>
</tbody>
</table>

Table 5.11: Inlet Manifold Pressure Metrics for Models 1-3

Figure 5.16 shows the results of the inlet manifold pressure when the discretized model is applied. Figure 5.16(a) shows that model 3 does not quite track the steady rise in inlet manifold pressure as well as Model 2. However, Fig. 5.16(b) shows that
the pressure spikes during each shift have been reduced, and are more similar in magnitude to the test data than Model 2 showed.

Table 5.11 confirms what is seen in Fig. 5.16. In general the performance has improved over Model 1, but interestingly Model 3 does not perform quite as well as Model 2.

**Exhaust Manifold Pressure of Model 3**

![Exhaust Manifold Pressure Graph](image)

(a) Results With Constant Load  
(b) Results With Shifting

Figure 5.17: Model 3 Exhaust Manifold Pressure Results

<table>
<thead>
<tr>
<th>Units</th>
<th>Constant Load</th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.075 Bar</td>
<td>0.044 Bar</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.026 Bar</td>
<td>0.025 Bar</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.021 Bar</td>
<td>0.021 Bar</td>
</tr>
</tbody>
</table>

Table 5.12: Exhaust Manifold Pressure Metrics for Models 1-3
The results of the exhaust manifold pressure for Model 3 are shown in Fig. 5.17. The results show the model does a fairly good job of tracking the exhaust manifold pressure during the constant current test, as seen in Fig. 5.17(a). In addition, Fig. 5.17 shows the pressure rise on each shift is well captured in Model 3. Table 5.12 shows that Model 3 does perform much better overall than Model 1, and in some metrics slightly better than Model 2.

Overall Model 3 shows fairly good performance in the modeling of the exhaust manifold pressure, but the inlet manifold pressure performance still needs some improvement. The examination of the pressure drop should help explain the differences between the inlet manifold and exhaust manifold pressure modeling performance.

**Cathode Pressure Drop of Model 3**

![Figure 5.18: Model 3 Pressure Drop Results](image)

Figure 5.18 explains why the exhaust manifold pressure from Model 3 performs better than the inlet manifold pressure does. As can be seen in Fig. 5.18(a), the
modeled pressure drop of the stack is relatively constant through out run, while the data shows a steady rise. As the pressure drop increases, the inlet manifold pressure should increase, but since the model does not capture the increase in the pressure drop, the inlet manifold pressure in Model 3 does not rise as much as it should. The reason the pressure drop does not rise much during the run, is that almost all the flow resistance is encountered upstream of the distributed model by a single linear resistance. Once full current draw is reached, the gases flowing through this resistance do not really change based on current draw or water production. The flow through the upstream stack resistance will always be that of humidified heliox. Therefor the upstream pressure drop should remain very constant because the composition and flow rate of gases won’t change much during full current testing conditions.

### 5.3.5 Model 3 Conclusions

An initial implementation of the discretized model has been analyzed. First a check of the model is performed by evaluating the number discretizations that should be used. Then the liquid water height and pressure drop characteristics of
the model are analyzed and shown to match reasonable expectations. Next the model-predicted outlet flow rate was compared to data, and the value of $\alpha$ equal to 1.0 was shown to match the test data well. Finally the pressure and pressure drop prediction of the model are analyzed.

It is shown that Model 3 provided better prediction of the exhaust manifold pressure. The results are better than model 2, because the model is better at providing a realistic water outlet flow rate. This new flow rate of liquid water flows through the two-phase back pressure valve model.

Model 3 performs poorly at predicting the pressure drop across the cathode. This is because the model only has a single upstream resistance. The pressure drop of the distributed model was shown to be practically negligible compared to the test data. The composition of the gases upstream of the stack will not change based on current draw or water production, so the pressure drop is relatively constant throughout the testing. Due to the lack of model-predicted pressure drop across the stack, the prediction of the inlet manifold pressure also suffers.

To address the problem of the stack pressure drop not reflecting the changing composition of gases, a second downstream stack resistance will be introduced in Model 4.

### 5.4 Discretized Model with a simple downstream resistance (Model 4)

In this section the discretized cathode model is used again to simulate the cathode water flow dynamics, but a downstream resistance is added to the overall model. The downstream resistance is added because Model 3 was failing to capture the total pressure drop of the cathode because its single resistance was upstream of the
cathode model, and did not change based on the composition of the gases. The simplified downstream resistance is a linearized pressure drop, where the total mass flow rate determined by the pressure difference is the sum of the liquid and gas flow rates.

5.4.1 Pressure Results of Model 4

In the following three sections the inlet manifold pressure, the exhaust manifold pressure, and the cathode pressure drop of Model 4 are analyzed. Table 5.14 shows the relevant calibration parameters used in the evaluation of Model 4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVT}P$</td>
<td>0.02</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$5.1e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>$6.3e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
</tbody>
</table>

Table 5.14: Calibration Parameters Model 4
Inlet Manifold Pressure of Model 4

Figure 5.19: Model 4 Inlet Manifold Pressure Results

<table>
<thead>
<tr>
<th>Units</th>
<th>Constant Load</th>
<th></th>
<th></th>
<th>Shifting</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
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<td>Mean Abs Err</td>
<td>Offset</td>
<td>Press.</td>
<td>Mean Abs Err</td>
<td>Offset</td>
<td>Press.</td>
<td>Pressure</td>
</tr>
<tr>
<td>Model 1</td>
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<td>0.068</td>
<td>0.152</td>
<td>0.112</td>
<td>0.066</td>
<td>0.172</td>
<td>0.177</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.041</td>
<td>0.039</td>
<td>0.033</td>
<td>0.057</td>
<td>0.090</td>
<td>0.049</td>
<td>0.322</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.067</td>
<td>0.039</td>
<td>0.055</td>
<td>0.074</td>
<td>0.049</td>
<td>0.057</td>
<td>0.126</td>
</tr>
<tr>
<td>Model 4</td>
<td>0.028</td>
<td>0.027</td>
<td>0.013</td>
<td>0.048</td>
<td>0.047</td>
<td>0.002</td>
<td>0.100</td>
</tr>
</tbody>
</table>

Table 5.15: Inlet Manifold Pressure Metrics for Models 1-4

Figure 5.19 shows significant improvement in the pressure prediction compared to Model 3, especially in the constant current test shown in Fig. 5.19(a). In the shifting case, seen in Fig. 5.19(b), the performance is also improved, as the low frequency rise in pressure is tracked, and the magnitude of the pressure spikes compares well
with the data. There is a pressure rise right at the end of the run predicted by the model, but not shown in the data. During this particular test, current was ramped down quickly because the heliox tank pressure was too low, and a quick shutdown was needed. This represents an unusual combination on unstable heliox flow and a transient in the current draw that the model is not able to capture.

Table 5.15 shows that Model 4 has the best performance of all the models for the pressure drop metrics. Relative to Model 3, every error metric has been reduced, and relative to the starting point of Model 1, all error metrics have been reduced significantly.

**Exhaust Manifold Pressure of Model 4**

![Exhaust Manifold Pressure Results](image)

Figure 5.20: Model 4 Exhaust Manifold Pressure Results

The performance of the exhaust manifold pressure is not expected to change with Model 4, since nothing related to the exhaust manifold was changed since Model 3. The results shown in Figure 5.20 confirm this, and show similar performance to
<table>
<thead>
<tr>
<th>Units</th>
<th>Mean Abs Err</th>
<th>Offset Error</th>
<th>Press. Rise Err</th>
<th>Mean Abs Err</th>
<th>Offset Error</th>
<th>Press. Rise Err</th>
<th>Pressure Spike Err</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>0.075</td>
<td>0.044</td>
<td>0.083</td>
<td>0.087</td>
<td>0.071</td>
<td>0.120</td>
<td>0.353</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.026</td>
<td>0.025</td>
<td>0.001</td>
<td>0.046</td>
<td>0.055</td>
<td>0.010</td>
<td>0.208</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.021</td>
<td>0.021</td>
<td>0.030</td>
<td>0.046</td>
<td>0.046</td>
<td>0.021</td>
<td>0.132</td>
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<tr>
<td>Model 4</td>
<td>0.022</td>
<td>0.021</td>
<td>0.020</td>
<td>0.045</td>
<td>0.045</td>
<td>0.015</td>
<td>0.149</td>
</tr>
</tbody>
</table>

Table 5.16: Exhaust Manifold Pressure Metrics for Models 1-4

Model 3 for both the constant current test and the shifting test. Table 5.16 confirms this by showing negligible change in the metrics between Model 3 and Model 4. Because the inlet manifold pressure modeling improved significantly between Model 3 and Model 4, while the exhaust manifold modeling remained the same, a great improvement in pressure drop prediction is expected.

**Cathode Pressure Drop of Model 4**

![Graph](image1)

(a) Results With Constant Load  

(b) Results With Shifting

Figure 5.21: Model 4 Pressure Drop Results
<table>
<thead>
<tr>
<th></th>
<th>Constant Load</th>
<th></th>
<th>Shifting</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
<td>Press. Rise Err</td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
<td>Press. Rise Err</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.045</td>
<td>0.029</td>
<td>0.069</td>
<td>0.038</td>
<td>0.044</td>
<td>0.052</td>
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<tr>
<td>Model 2</td>
<td>0.019</td>
<td>0.019</td>
<td>0.031</td>
<td>0.024</td>
<td>0.040</td>
<td>0.060</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.056</td>
<td>0.033</td>
<td>0.085</td>
<td>0.051</td>
<td>0.012</td>
<td>0.036</td>
</tr>
<tr>
<td>Model 4</td>
<td>0.014</td>
<td>0.015</td>
<td>0.033</td>
<td>0.013</td>
<td>0.013</td>
<td>0.013</td>
</tr>
</tbody>
</table>

Table 5.17: Pressure Drop Metrics for Models 1-4

Since the changes implemented for Model 4 were mainly related to capturing the pressure drop, the most significant change between Model 3 and Model 4 should be seen in the pressure drop results. Figure 5.21 shows a significant improvement. Because two separate resistances are used to obtain the total pressure drop of the cathode, the plot shows the $\Delta P$ of both the upstream and downstream resistances, as well as the total $\Delta P$.

In Fig. 5.21(a) the model shows excellent correlation with the test results during constant current operation. It can be seen that the upstream resistance was lowered relative to Model 3, but again remains relatively constant throughout the run. The downstream resistance however, which accounts for increased water flow, slowly rises over the run and captures the increase in $\Delta P$.

For the shifting case seen in Fig. 5.21(b), the model is generally good at capturing the low frequency characteristics. The model does however show small pressure spikes for each shift that are not seen in the data, although they are reduced significantly from the pressure drop spikes seen in Models 1 and 2.
Table 5.17 confirms the improved performance of the pressure drop modeling of Model 4. In almost all metrics Model 4 shows the best performance, or negligible differences from another model.

5.4.2 Model 4 Conclusions

Model 4 showed an improvement over Model 3 mainly in the prediction of the pressure drop across the stack. Because the stack resistance was split into an upstream and downstream resistance, the downstream resistance was able to account for an increased flow resistance related to the increase in liquid water outlet flow rate. Because the pressure drop of the stack was modeled with more accuracy, the inlet manifold pressure also showed an increased match with the data.

5.5 Discretized Model with a Two Phase Downstream Resistance (Model 5)

The results of this section are for Model 5, which is fairly similar to Model 4. The model continues to use the discretized cathode model to predict the exit water flow characteristics, and adds a downstream resistance. The downstream resistance used in this model, however, is a recommended equation from a text on two-phase flow, instead of a simplified linear resistance. It is hoped this will help improve the performance of the model.

5.5.1 Pressure Results of Model 5

The following section provides the pressure results of Model 5. Again, the inlet manifold pressure, exhaust manifold pressure, and cathode pressure drop will be investigated. In all cases the performance of Models 4 and 5 are nearly identical.
Table 5.18 shows the relevant calibration parameters that were used in the evaluation of Model 5.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
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<td>$P_{\text{preset}}$</td>
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<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVT}$</td>
<td>0.02</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$4.6e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>2100</td>
<td>$1/(m^2kg)$</td>
</tr>
</tbody>
</table>

Table 5.18: Calibration Parameters Model 5

Inlet Manifold Pressure of Model 5

Figure 5.22 shows the inlet manifold pressure of Model 5. Its performance is nearly identical to Model 4, which is confirmed by the negligible change in the metrics as seen in Table 5.19.

Figure 5.22: Model 5 Inlet Manifold Pressure Results
### Table 5.19: Inlet Manifold Pressure Metrics for Models 1-5

<table>
<thead>
<tr>
<th>Units</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
<th>Bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Abs Err</td>
<td>0.119</td>
<td>0.068</td>
<td>0.152</td>
<td>0.112</td>
<td>0.066</td>
<td>0.172</td>
<td>0.177</td>
<td></td>
</tr>
<tr>
<td>Offset Error</td>
<td>0.041</td>
<td>0.039</td>
<td>0.033</td>
<td>0.057</td>
<td>0.090</td>
<td>0.049</td>
<td>0.322</td>
<td></td>
</tr>
<tr>
<td>Press. Rise Err</td>
<td>0.067</td>
<td>0.039</td>
<td>0.055</td>
<td>0.074</td>
<td>0.049</td>
<td>0.057</td>
<td>0.126</td>
<td></td>
</tr>
<tr>
<td>Mean Abs Err</td>
<td>0.028</td>
<td>0.027</td>
<td>0.013</td>
<td>0.048</td>
<td>0.047</td>
<td>0.002</td>
<td>0.100</td>
<td></td>
</tr>
<tr>
<td>Offset Error</td>
<td>0.030</td>
<td>0.029</td>
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<td>0.050</td>
<td>0.002</td>
<td>0.088</td>
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<tr>
<td>Press. Rise Err</td>
<td>0.067</td>
<td>0.039</td>
<td>0.055</td>
<td>0.074</td>
<td>0.049</td>
<td>0.057</td>
<td>0.126</td>
<td></td>
</tr>
<tr>
<td>Spike Err</td>
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<td>0.100</td>
<td>0.100</td>
<td>0.088</td>
<td>0.088</td>
<td></td>
</tr>
</tbody>
</table>

Exhaust Manifold Results of Model 5

Figure 5.23 shows the exhaust manifold performance of Model 5. Similar to the inlet manifold performance, the performance of Model 4 and 5 are practically indistinguishable.
### Table 5.20: Exhaust Manifold Pressure Metrics for Models 1-5

<table>
<thead>
<tr>
<th>Model</th>
<th>Constant Load</th>
<th>Shifting</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean Abs Err</td>
<td>Offset Error</td>
</tr>
<tr>
<td>Units</td>
<td>Bar</td>
<td>Bar</td>
</tr>
<tr>
<td>Model 1</td>
<td>0.075</td>
<td>0.044</td>
</tr>
<tr>
<td>Model 2</td>
<td>0.026</td>
<td>0.025</td>
</tr>
<tr>
<td>Model 3</td>
<td>0.021</td>
<td>0.021</td>
</tr>
<tr>
<td>Model 4</td>
<td>0.022</td>
<td>0.021</td>
</tr>
<tr>
<td>Model 5</td>
<td>0.022</td>
<td>0.021</td>
</tr>
</tbody>
</table>

### Cathode Pressure Drop of Model 5

![Figure 5.24: Model 5 Pressure Drop Results](image)

(a) Results With Constant Load  
(b) Results With Shifting

Figure 5.24 shows the cathode pressure drop of Model 5. The total pressure drop of Model 4 and Model 5 are nearly identical. The only real difference is that through calibration, the upstream resistance was increased slightly in Model 5, resulting in the upstream pressure drop being only .02 bar higher than in Model 4. The metrics
Table 5.21: Pressure Drop Metrics for Models 1-5

Presented in Table 5.21 confirm that there are negligible performance differences between Models 4 and 5.

5.5.2 Model 5 Conclusions

Model 5 shows nearly identical performance in almost every aspect compared to Model 4. Since the model is based on a more accepted method of predicting pressure drop for two phase flow, and its downstream resistance is not a linearized pressure drop, it will be chosen as the best, since it would likely be adaptable to a wider range of operating conditions without needing recalibration.

5.6 Model Calibration

Model 5 depends on five different tunable parameters to adjust the model to perform similar to the test data. This section details how each of the parameters is individually tuned so the model will perform properly. For some parameters test data under constant current is examined during calibration, while for others the
data with shifting is examined. To start off, the results of a “poorly calibrated” model simulation are shown to provide a reference starting point.

5.6.1 Pressure Results of a Poorly Calibrated Model

The following three subsections show the inlet manifold pressure, exhaust manifold pressure, and cathode pressure drop of a poorly calibrated model to give a reference as the model is tuned to match the test data. Table 5.22 shows the parameters used in the model to show the results of the poorly calibrated model.

<table>
<thead>
<tr>
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<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
<td>24</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>$K_{BPVTOP}$</td>
<td>0.0</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$6.96e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>Not Used</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.22: Calibration Parameters For a Poorly Tuned Model (Step 0)
Inlet Manifold Pressure of Poorly Calibrated Model

Figure 5.25: Poorly Calibrated Inlet Manifold Pressure Results

Figure 5.25 shows the results of the inlet manifold pressure with the poorly calibrated model compared to the test data. As can be seen, the inlet manifold pressure is too low overall, does not increase at all as the run progresses, and shows almost no rise during vehicle shifts. In fact, the y-axis of these plots had to be changed from the standard used for all the other results presented in this dissertation because the inlet pressure simply stayed out of the range of the normal plot scale.
Exhaust Manifold Pressure of Poorly Calibrated Model

Figure 5.26: Poorly Calibrated Exhaust Manifold Pressure Results

Figure 5.26 shows the exhaust manifold pressure from the poorly tuned model compared to the test data. Again, the overall operating pressure is too low, there is no increase at all as the run progresses, and there are negligible pressure increases with each shift. The fact the exhaust manifold pressure is too low is a part of the reason why the inlet manifold pressure is also too low, the other reason will be shown by the cathode pressure drop.
Figure 5.27 shows the pressure drop of the cathode for the poorly calibrated model compared to the test data. The overall pressure drop is far too low, and does not increase at all over the length of the run. The inlet manifold pressure is far too low because of the combined effects from the cathode pressure drop being too low, and the exhaust manifold pressure being too low.

5.6.2 Calibrating the Back Pressure Valve Setting $P_{\text{preset}}$
(Step 1)

The BPV pressure setting is the first calibration parameter adjusted, as it grossly affect the exhaust manifold pressure, and therefor the inlet manifold pressure. In Step 1 of model calibration, the back pressure valve preset is changed. Table 5.23 shows the parameters used in step 1 of the calibration.
Table 5.23: Calibration Parameters For Step 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>1.0</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.0</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$6.96e^{-6}$</td>
<td>$kg/(Pa \cdot s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>Not Used</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.28: Step 1, Calibrating the Back Pressure Valve Setting $P_{\text{preset}}$

Figure 5.28 shows the before and after effects of increasing the back pressure valve setting. The best plot to look at for the results is the exhaust manifold pressure during a constant current test. Increasing the valve setting raises the exhaust manifold pressure closer to the pressure seen in the test data, particularly early in the test. The model at this stage in calibration still fails to show a pressure rise over the length of the test.
5.6.3 Calibrating the Back Pressure Restriction $K_{BPV}$ (Step 2)

As mentioned in Chapter 3, after creating the back pressure valve model from the manufacturers data, it was found that the valve in practice was more restrictive than the data sheet. Particularly it was found in practice the valve was far more sensitive to the composition and flow rate changes during shifting transients than simple calculations from the data sheet implied. To make the valve more sensitive to the gas composition and flow rate changes, the tunable parameter $K_{BPV}$ was introduced and can be adjusted to show a more realistic response from the back pressure valve.

Step 2 of the calibration is the adjustment of $K_{BPV}$ to reflect the valves sensitivity to shifting transients. Table 5.24 shows the new parameters used in step 2 of the calibration. Viewing the exhaust manifold pressure from a test with shifting transients is the best way to adjust this parameter.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{preset}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.0</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{us}$</td>
<td>$6.96 \times 10^{-6}$</td>
<td>$kg/(Pa \cdot s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>Not Used</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.24: Calibration Parameters For Step 2
Figure 5.29: Step 2, Calibrating the Back Pressure Restriction $K_{BPV}$

Figure 5.29 compares the effect of changing the parameter $K_{BPV}$. As the figure shows, before this parameter is adjusted the valve shows almost no sensitivity to the shifting transients. After the adjustment the pressure is seen to spike during each shift.

5.6.4 Calibrating the Back Pressure Valve Two Phase Restriction $K_{BPVT}$ (Step 3)

Step 3 of the model calibration deals with adjusting the back pressure valves sensitivity to the two phase flow. This parameter, $K_{BPVT}$, adjusts how much the calculated $C_dA$ is reduced based on the water content in the exhaust manifold. Table 5.25 shows the parameters after they have been adjusted for tuning step 3. To adjust this parameter the exhaust pressure during a constant current test is the best variable to view.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{preset}$</td>
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<td>psi</td>
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<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.02</td>
<td>m$^2$/kg</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$6.96e^{-6}$</td>
<td>kg/(Pa·s)</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>Not Used</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.25: Calibration Parameters For Step 3

Figure 5.30: Step 3, Calibrating the Back Pressure Valve Two Phase Restriction $K_{BPVTP}$

Figure 5.30 shows the exhaust manifold pressure for a constant current test, before and after the parameter $K_{BPVTP}$ has been adjusted. The results show that the exhaust manifold pressure now tracks the test data well throughout the length of the run, because the back pressure valve is sensitive to the increase in liquid water flow rate throughout the run.
5.6.5 Calibrating the Upstream Flow Resistance $K_{US}$ (Step 4)

The 4th step in the calibration is the adjustment of the upstream flow resistance. This flow resistance needs to be increased, as the initial pressure drop was far too low. However, it cannot be increased too much, because a second downstream resistance will be added, and the sum of the two will equal the total pressure drop across the cathode. Table 5.26 shows the parameters adjusted for the 4th step of the calibration. Note that to increase the flow resistance, the value of $K_{US}$ actually has to be reduced numerically. The best method to evaluate this change is to view the cathode pressure drop during a constant current test.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{preset}$</td>
<td>30</td>
<td>psi</td>
</tr>
<tr>
<td>$K_{BPV}$</td>
<td>0.25</td>
<td>N/A</td>
</tr>
<tr>
<td>$K_{BPVTP}$</td>
<td>0.02</td>
<td>$m^2/kg$</td>
</tr>
<tr>
<td>$K_{US}$</td>
<td>$4.64e^{-6}$</td>
<td>$kg/(Pa \cdot s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>Not Used</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.26: Calibration Parameters For Step 4
Figure 5.31: Step 4, Calibrating the Upstream Flow Resistance $K_{US}$

Figure 5.31 shows the results before and after $K_{US}$ has been adjusted. As the plot shows, the stack resistance is increase, showing a higher $\Delta P$ after the change. The stack resistance is still incapable of capturing the rise in pressure drop as the run progresses, because there is no downstream resistance that is taking into account the two phase flow.

### 5.6.6 Calibrating the Downstream Flow Resistance $K_{DS}$ (Step 5)

The final step in the calibration procedure is the implementation and calibration of the two-phase downstream resistance. This will affect the cathode pressure drop response in relation to changes in liquid outlet flow rate. Table 5.27 shows the parameters implemented for Step 5 of the calibration procedure. Similar to Step 4, the cathode pressure drop during a constant current test provides the best method to tune this parameter.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>$P_{\text{preset}}$</td>
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<td>$K_{BPV}$</td>
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<td>$K_{BPVTP}$</td>
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<tr>
<td>$K_{US}$</td>
<td>$4.64e^{-6}$</td>
<td>$kg/(Pa - s)$</td>
</tr>
<tr>
<td>$K_{DS}$</td>
<td>2100</td>
<td>$1/(m^2kg)$</td>
</tr>
</tbody>
</table>

**Table 5.27: Calibration Parameters For Step 5**

Figure 5.32 shows the results before and after the downstream resistance is implemented and calibrated. As the results show, the downstream resistance allows the cathode pressure drop to track the rise in the pressure drop as the test run progresses. The performance of the rest of the model to both shifting and steady state testing has already been shown in Section 5.5, as the calibration parameters have now been tuned to match those used in Model 5.
5.6.7 Calibration Conclusions

This section highlighted the tuning procedure used, specifically related to Model 5, although the general procedure was followed for Models 1-5, where their parameters were applicable. The five tunable parameters need to be adjusted to capture specific effects of the model. The first step starts with the simplest parameter, $P_{\text{preset}}$, and the operating pressure of the system is adjusted. In step 2, $K_{BPV}$ is used to adjust the sensitivity of the back pressure valve to changes in flow rate and composition during shifts. Step 3 adjusts $K_{BPVTP}$ to adjust how the back pressure valve responds to increasing outlet flow rate of liquid water as the test run progresses. In Step 4, $K_{US}$ is adjusted to account for the upstream flow resistance of the stack to the incoming flow rate. Finally, Step 5 adjusts $K_{DS}$ to account for the flow resistance through the downstream portion of the stack, and its sensitivity to the changing two-phase composition as more liquid water exits throughout the run.

5.7 Model 5 Applied to Race Data

The previous sections detailed the development and tuning of the cathode model based on data from static testing. To test the model performance in non lab conditions, it is used with actual vehicle race data to see how closely the performance matches the model.

The system used in the race conditions will have a few dissimilarities compared to the model used. When the vehicle was put in race conditions, the cathode PRV’s were tuned to be very close to the cathode operating pressure. They were tuned so close that it is likely that there was even leakage flow during parts of the run.
For the test stand data presented earlier in this chapter, the PRV’s were adjusted to a very high setting so they would be inactive during the test.

Additionally, the back pressure valve settings are slightly different between the two sets. When the static testing was completed after the Bonneville race, the operating pressure was increased slightly to ensure stable high power operation for the constant current run.

5.7.1 Pressure Results of Uncalibrated Model 5 with Race Data

Initial results are presented with the model calibrations equal to those seen in Model 5. As mentioned, some discrepancies in performance are expected due to the un-modeled PRV’s, and the slightly different back pressure valve settings. Results are again presented for the inlet manifold pressure, the exhaust manifold pressure, and the cathode pressure drop. Table 5.28 shows that the calibration parameters used in this initial evaluation of the race data are the same that were used in Model 5 when presented previously.

<table>
<thead>
<tr>
<th>Parameter</th>
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<td>$m^2/kg$</td>
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<td>$4.64e^{-6}$</td>
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</tr>
<tr>
<td>$K_{DS}$</td>
<td>2100</td>
<td>$1/(m^2kg)$</td>
</tr>
</tbody>
</table>

Table 5.28: Calibration Parameters Model 5 with race data
Figure 5.33: Inlet Manifold results of new model applied to race data.

Figure 5.33 shows the results of the inlet manifold pressure when Model 5 is applied to the race data model without any calibration changes. As expected due to slightly different back pressure valve settings, the operating pressure is higher than the data shows.
Figure 5.34: Exhaust Manifold results of new model applied to race data.

Figure 5.34 shows the results of the exhaust manifold pressure when Model 5 is applied to the race data without any calibration changes. As already mentioned, the slightly higher BPV valve setting leads to a higher back pressure in the model when compared to the test data.
Figure 5.35: Pressure Drop results of new model applied to race data.

Figure 5.35 shows the stack pressure drop of Model 5 with no calibration changes when applied to the race data. Here we would not expect to see any performance differences in an ideal case. Unfortunately there are a few discrepancies that can most likely be explained by the PRV’s that were active in the race, but not modeled in Model 5.

First, the test data actually shows a dip in the pressure drop across the stack during shifts, while the model actually shows a small increase in the pressure drop. The test data dip in pressure drop is actually a relic of the PRV’s venting during a shift, where the upstream pressure is lowered due to the PRV.
The second discrepancy seen is that the low frequency performance of the pressure drop by the model predicts a slightly higher pressure drop than the test data shows. This is also likely explained by the PRV’s. Through the careful testing and tuning of the system detailed in Chapter 4, the PRV’s were set very close to the peak operating pressure of the stack. In fact, its likely they were actually providing a trace leakage amount continuously throughout the run. With a slight leakage upstream of the stack, we would expect less flow to go through the upstream and downstream resistance, which the model cannot predict.

5.7.2 Pressure Results of Calibrated Model 5 with Race Data

With a few small changes to the calibration parameters, the model performance can be improved. The upstream stack resistance is lowered slightly, and the back pressure valve setting is increased a minimal amount. Table 5.29 shows the slight modifications made to the Model 5 calibrations to more closely match the race data.

<table>
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<td>$K_{BPVTP}$</td>
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<td>$m^2/kg$</td>
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<tr>
<td>$K_{US}$</td>
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</tr>
<tr>
<td>$K_{DS}$</td>
<td>2000</td>
<td>$1/(m^2kg)$</td>
</tr>
</tbody>
</table>

Table 5.29: Modified Calibration Parameters for Model 5 with Race Data
Inlet Manifold Pressure of Calibrated Model 5

Figure 5.36: Inlet Manifold results of new model with changed calibrations applied to race data.

Figure 5.36 shows the inlet manifold pressure after the back pressure setting and pressure drop have been recalibrated. The performance of the model lines up very well with the data.
Exhaust Manifold Pressure of Calibrated Model 5

Figure 5.37: Exhaust Manifold results of new model with changed calibrations applied to race data.

Figure 5.37 shows the exhaust manifold pressure of the model after it has been recalibrated. The model performance also corresponds with the test data.
Figure 5.38 shows the cathode pressure drop after the model has been recalibrated. After lowering the upstream and downstream resistances slightly to reflect the trace flow that might be escaping through the PRV’s, the modeled pressure drop lines up quite well with the test data. The model still predicts pressure drop increases during shifting, while the test data shows dips in the pressure drop. This is again due to the action of the PRV, which is not captured in the model.

5.7.3 Model 5 Applied to Race Data Conclusions

The results of this section show that the model, when calibrated from the test data, does not match up exactly with the data from the BB2 race event. The
difference in back pressure is quickly adjusted by adjusting the preset BPV setting, which was a known physical difference between the two sets of data.

The pressure drop of the stack however, needed some calibration changes that were not expected. However, the fact the PRVs were active during race events, but not modeled in Model 5 might explain the differences. With trace outlet flow from the PRV’s, there would be less gas passing through the cathode, leading to a lower pressure drop. Also the dips in pressure drop seen in the data are a result of the PRV’s opening with each shift, a phenomenon that isn’t captured in Model 5.

5.8 Modeling Conclusions and Future Work

The results shown in this chapter provided a significant improvement in the modeling of the pressure dynamics of the BB2 fuel cell system. Notable improvements were made in both the transient pressure prediction during shifts, and the more constant pressure dynamics during a sustained long term test. The improvements were found mainly through the adjustment of the tunable parameters that were sensitive to the outlet flow rate of liquid water predicted by the discretized model. Despite the remarkable improvement, there are several areas where future work could be considered.

The discretized model wound up showing excellent correlation with the data for the tests conducted on the BB2 system, which were a ramp up to full power operation, sometimes interrupted by shifts. While this provided a great improvement, it does not provide any indication on how the discretized mode would perform in steps down in current. The BB2 only really cares about attaining peak power, but
other fuel cell systems would be required to run at a variety of power levels, and it is unclear how the discretized model would perform stepping down in current draw.

The model still showed some areas in the exhaust manifold and intake manifold pressure where the pressure prediction was not exact. There were notable areas between the shifting transients, where the pressure would vary, but the model would not reflect this. Due to the excellent performance of the pressure drop, and the fact that errors were seen in the exhaust pressure and the intake pressure, its likely this error is due to the back pressure valve model. The back pressure valve model used in the this work was a static model, despite the fact the valve uses a spring and pitot tube. It is likely some dynamics could be included in the valve model that might explain the performance. A better back pressure valve model could possibly be built through more bench testing, with transient flow, and two-phase flow conditions.

However, the back pressure valve used in the BB2 was a passive device, that was difficult to test and tune. Its likely for a more robust system with better control, a different method of controlling back pressure would be needed. In fact, if the BB2 were able to be run for another year, these modeling efforts would be used to help design a control algorithm for a new back pressure device to avoid the transient pressure spikes seen in the BB2.

In the final model, Model 5, the upstream resistance used was a linearized resistance. This was not changed from Model 1 due to the relatively constant operating conditions experienced by the BB2. If the model needed to be extended to other operating conditions, a nonlinear expression for the upstream resistance could easily be incorporated, or a scheduled model with a variety of linearized resistances could also be used. The downstream resistance used was a non linear model, but
It's possible it might also need to have a scheduled model applied to improve the downstream pressure drop modeling during a larger variety of operating conditions.

The metrics proved to be a fairly accurate method of evaluating the relative performance of the models. Depending on what performance characteristics were most desirable to the system designer, weights could be added to these error metrics to create an overall score for the model performance. Then using the metrics, an automated routine could be used to do model calibration, rather than a manual adjustment followed by evaluation. This could easily be implemented as well at a variety of operating conditions to create a scheduled model of calibration parameters.

### 5.9 Chapter Conclusion

This chapter provided the results of the cathode pressure modeling efforts for the BB2 system. The first results presented were those of the control oriented model adapted from [60] to match the BB2 system layout. This model does not deal with liquid water, and therefore showed poor predictive ability when used with the BB2, which operates at extremely high current density where significant water production is present.

Next a simple adaptation of this model to deal with two phase flow was introduced, and showed some improvement in a few areas of the pressure dynamics, giving further credit to the need to consider the liquid water.

Then the discretized laminar flow model developed in Chapter 3 was applied, and model performance was further improved, except for in the area of pressure drop across the stack. It was found that the discretized model, with only an upstream
flow resistance, could not accurately capture the rise in pressure drop as more and more liquid water exited the stack as the run progressed.

To further improve the modeling of the pressure drop, an resistance was added downstream of the cathode channels. This resistance was first added using a simplified method of dealing with two phase flow, and secondly with a published relation for the pressure drop of two phase flow through a restriction. The performance of these models showed a significant improvement in the overall pressure drop modeling of the stack.

Additionally a section on model calibration was provided, to show progressively how each parameter affects the performance of the model. Finally the model was applied to race data. Because of a few discrepancies between the system used for the race conditions, and the test data used in model development, the model calibrations had to be slightly adjusted, and then the model performed very well compared to the race data.


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APPENDIX A

Flow Derivation without Slip

A.1 Flow Derivation without Slip

A.1.1 Equations for Lower Fluid

For the Lower Fluid, the generic Velocity equation is

\[ u = \frac{1}{2\mu} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_1}{\mu} y + c_2 \]

With more specific naming convention per the diagram above

\[ u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_{1L}}{\mu_L} y + c_{2L} \]

Boundary Conditions

@\( y = 0 \), \( u_L = 0 \)
@\( y = h \), \( u_L = V \)

From first boundary condition

\[ c_{2L} = 0 \]

And velocity equation becomes. Change \( c_{1L} \) to simply \( c_L \)

\[ u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_L}{\mu_L} y \]

From Second boundary Condition

\[ V = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h \]
A.1.2 Equations for Upper Gas

For the Lower Fluid, the generic equation is

\[ u = \frac{1}{2\mu} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_1}{\mu} y + c_2 \]

With more specific naming convention per the diagram above.

\[ U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_{1g}}{\mu_g} Y + c_{2g} \]

Boundary Conditions

@Y = 0, U_L = 0
@Y = H, U_L = V

From first boundary condition

\[ c_{2g} = 0 \]

And velocity equation becomes. Change \( c_{1g} \) to simply \( c_g \)

\[ U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_g}{\mu_g} Y \]

From Second boundary Condition

\[ V = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{c_g}{\mu_g} H \]
A.1.3 Shear Stress of Lower Fluid

Shear Stress Distribution for a Newtonian fluid is given by

\[ \tau_{yx} = \mu_L \left( \frac{du_L}{dy} \right) \]

Plug Velocity Eqn \((\cdot)\) in, drop \(C_{2L}\)

\[ \tau_{yx} = \mu_L \left( \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{C_L}{\mu_L} y \right) \]

Evaluate the derivative

\[ \tau_{yx} = \left( \frac{\partial p}{\partial x} \right) y + \frac{C_L}{\mu_L} \]

Evaluated @ \(y=h\)

\[ \tau_{yx}|_{y=h} = \left( \frac{\partial p}{\partial x} \right) h + \frac{C_L}{\mu_L} \]

A.1.4 Shear Stress of Upper Gas

Shear Stress Distribution for a Newtonian fluid is given by

\[ \tau_{yx} = \mu_g \left( \frac{dU_g}{dY} \right) \]

Plug Velocity Eqn \((\cdot)\) in, drop \(C_{2L}\)

\[ \tau_{yx} = \mu_g \left( \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{C_g}{\mu_g} Y \right) \]

Evaluate the derivative

\[ \tau_{yx} = \left( \frac{\partial p}{\partial x} \right) Y + \frac{C_g}{\mu_g} \]

Evaluated @ \(Y=H\)

\[ \tau_{yx}|_{Y=H} = \left( \frac{\partial p}{\partial x} \right) H + \frac{C_g}{\mu_g} \]
Set Shear Stresses equal to each other. Eqns 5 and 6

$$\left( \frac{\partial p}{\partial x} \right)_h + c_L = \left( \frac{\partial p}{\partial x} \right)_H + c_g$$

Thus We have 3 unknowns V, cL and cg and the following 3 equations

$$V = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right)_h^2 + \frac{c_L}{\mu_L} h$$

$$V = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)_H^2 + \frac{c_g}{\mu_g} H$$

$$\left( \frac{\partial p}{\partial x} \right)_h + c_L = \left( \frac{\partial p}{\partial x} \right)_H + c_g$$

Solve Equation 7 for cg

$$c_g = \left( \frac{\partial p}{\partial x} \right)_h + c_L - \left( \frac{\partial p}{\partial x} \right)_H$$

Set 2 and 4 equal to each other

$$\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right)_h^2 + \frac{c_L}{\mu_L} h = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)_H^2 + \frac{c_g}{\mu_g} H$$
Insert Eqn 8 into 9 and solve for $c_L$

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{H}{\mu_g} \left[ \left( \frac{\partial p}{\partial x} \right) h + c_L - \left( \frac{\partial p}{\partial x} \right) H \right]
\]

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{H}{\mu_g} c_L - \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) H
\]

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{H}{\mu_g} c_L - \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

\[
\frac{h}{\mu_L} c_L - \frac{H}{\mu_g} c_L = \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) h - \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2
\]

\[
c_L \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right] = \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{2H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2
\]

\[
c_L \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right] = + \frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

\[
c_L = \frac{\frac{H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)}{\left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]}
\]
Insert Eqn (1) into Eqn 8 and solve for \( c_g \)

\[
c_g = \left( \frac{\partial p}{\partial x} \right) h + \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H
\]

\[
c_g = \frac{\left( \frac{\partial p}{\partial x} \right) h}{h - H} \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \left( \frac{\partial p}{\partial x} \right) h \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right] + \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \frac{\left( \frac{\partial p}{\partial x} \right) h}{h - H} \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \frac{h^2}{\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{H^2}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \frac{\left( \frac{\partial p}{\partial x} \right) h}{h - H} \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{H^2}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{H}{\mu_g} \right]
\]

\[
c_g = \frac{h^2}{\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{H^2}{\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

\[
c_g = \frac{h}{\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]
The Liquid constant from equation 10 can be rewritten as:

\[ c_L = \frac{Hh}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) \]

\[ c_L = \frac{Hh}{\mu_g} - \frac{h^2}{2\mu_L} + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) = CC_L \left( \frac{\partial p}{\partial x} \right) \]

Where

\[ CC_L = \frac{Hh}{\mu_g} - \frac{h^2}{2\mu_L} + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) \]

The Gas constant from equation 11 can be rewritten as:

\[ c_g = \frac{-Hh}{\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) \]

\[ c_g = \frac{-Hh}{\mu_L} + \frac{h^2}{2\mu_L} + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) = CC_g \left( \frac{\partial p}{\partial x} \right) \]

Where

\[ CC_g = \frac{-Hh}{\mu_L} + \frac{h^2}{2\mu_L} + \frac{H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) \]
Velocity Profiles from Equations 1 and 3 can be rewritten using $DL$ and $Dg$. The liquid velocity

$$u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{D_L}{\mu_L} \left( \frac{\partial p}{\partial x} \right) y$$

$$u_L = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_L} y^2 + \frac{D_L}{\mu_L} y \right]$$

The gas velocity

$$U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{D_g}{\mu_g} \left( \frac{\partial p}{\partial x} \right) Y$$

$$U_g = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_g} Y^2 + \frac{D_g}{\mu_g} Y \right]$$
A.1.5 Liquid Volumetric Flow Rate

Now integrate velocity profile to attain volumetric flow rate.

\[ Q = \int_A \vec{V} \cdot d\vec{A} \]

For the liquid with channel width of \( a \)

\[ Q_L = \int_0^h u_L dy \]

\[ \frac{Q_L}{a} = \int_0^h u_L dy \]

\[ \frac{Q_L}{a} = \int_0^h \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_L} y^2 + \frac{D_L}{\mu_L} y \right] dy \]

\[ \frac{Q_L}{a} = \left( \frac{\partial p}{\partial x} \right) \int_0^h \left[ \frac{1}{2\mu_L} y^2 + \frac{D_L}{\mu_L} y \right] dy \]

\[ \frac{Q_L}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{D_L}{2\mu_L} h^2 \right]_0^h \]

\[ Q_L = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{D_L}{2\mu_L} h^2 \right] \]
A.1.6 Gas Volumetric Flow Rate

Now integrate velocity profile to attain volumetric flow rate.

\[ Q = \int_A \vec{V} \cdot d\vec{A} \]

For the gas with channel width of \( a \)

\[ Q_g = \int_0^H U_g dY \]

\[ \frac{Q_g}{a} = \int_0^H U_g dY \]

\[ \frac{Q_g}{a} = \int_0^H \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_g} Y^2 + \frac{D_g Y}{\mu_g} \right] dY \]

\[ \frac{Q_g}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_g} Y^3 + \frac{D_g Y^2}{2\mu_g} \right]_0^H \]

\[ \frac{Q_g}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{D_g H^2}{2\mu_g} \right] \]
A.1.7 Summary

The Liquid Volumetric Flow Rate is given by:

\[ \frac{Q_L}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6 \mu_L} h^3 + \frac{CC_L h^2}{2 \mu_L} \right] \]

Where

\[ CC_L = \frac{H h}{\mu_g} - \frac{h^2}{2 \mu_L} - \frac{H^2}{2 \mu_g} \]

The Gas Volumetric Flow Rate is given by:

\[ \frac{Q_g}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6 \mu_g} H^3 + \frac{CC_g H^2}{2 \mu_g} \right] \]

Where

\[ CC_g = \frac{H h}{\mu_L} + \frac{h^2}{2 \mu_L} + \frac{H^2}{2 \mu_g} \]
APPENDIX B

Flow Derivation with slip

B.1 Flow Derivation with slip

B.1.1 Equations for Lower Fluid

For the Lower Fluid, the generic Velocity equation is

\[ u = \frac{1}{2\mu} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_1}{\mu} y + c_2 \]

With more specific naming convention per the diagram above

\[ u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_{1L}}{\mu_L} y + c_{2L} \]

Boundary Conditions

\[ @y = 0, u_L = 0 \]
\[ @y = h, u_L = V \]

From first boundary condition

\[ c_{2L} = 0 \]

And velocity equation becomes. Change c1L to simply cL

\[ u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_L}{\mu_L} y \]

From Second boundary Condition

\[ V = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h \]
B.1.2 Equations for Upper Gas

For the Lower Fluid, the generic equation is

\[ u = \frac{1}{2\mu} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_1}{\mu} y + c_2 \]

More with more specific naming convention per the diagram above.

\[ U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_{1g}}{\mu_g} Y + c_{2g} \]

Boundary Conditions

@Y = 0, U_L = 0
@Y = H, U_L = V

From first boundary condition

\[ c_{2g} = 0 \]

And velocity equation becomes. Change c1g to simply cg

\[ U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_g}{\mu_g} Y \]

From Second boundary Condition

\[ V = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{c_g}{\mu_g} H \]
B.1.3 Shear Stress of Lower Fluid

Shear Stress Distribution for a Newtonian fluid is given by

$$\tau_{yx} = \mu_L \left( \frac{du_L}{dy} \right)$$

Plug Velocity Eqn () in, drop C2L

$$\tau_{yx} = \mu_L \left( \frac{d}{dy} \left( \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{c_L}{\mu_L} Y \right) \right)$$

Evaluate the derivative

$$\tau_{yx} = \mu_L \left( \frac{2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) Y + \frac{c_L}{\mu_L} \right)$$

$$\tau_{yx} = \left( \frac{\partial p}{\partial x} \right) Y + c_L$$

Evaluated @ $y=h$

$$\tau_{yx} \bigg|_{y=h} = \left( \frac{\partial p}{\partial x} \right) h + c_L$$

B.1.4 Shear Stress of Upper Gas

Shear Stress Distribution for a Newtonian fluid is given by

$$\tau_{yx} = \mu_g \left( \frac{dU_g}{dY} \right)$$

Plug Velocity Eqn () in, drop C2L

$$\tau_{yx} = \mu_g \left( \frac{d}{dY} \left( \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{c_g}{\mu_g} Y \right) \right)$$

Evaluate the derivative

$$\tau_{yx} = \mu_g \left( \frac{2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y + \frac{c_g}{\mu_g} \right)$$

$$\tau_{yx} = \left( \frac{\partial p}{\partial x} \right) Y + c_g$$

Evaluated @ $Y=H$

$$\tau_{yx} \bigg|_{Y=H} = \left( \frac{\partial p}{\partial x} \right) H + c_g$$

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Set Shear Stresses equal to each other. Eqns 5 and 6

\[ \left( \frac{\partial p}{\partial x} \right) h + c_L = \left( \frac{\partial p}{\partial x} \right) H + c_g \]

Thus We have 3 unknowns V, cL and cg and the following 3 equations

\[ V_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h \quad \text{with unkowns of } V \text{ and } c_L \]

\[ V_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{c_g}{\mu_g} H \quad \text{with unkowns of } V \text{ and } c_g \]

\[ \left( \frac{\partial p}{\partial x} \right) h + c_L = \left( \frac{\partial p}{\partial x} \right) H + c_g \]

Solve Equation 7 for cg

\[ c_g = \left( \frac{\partial p}{\partial x} \right) h + c_L - \left( \frac{\partial p}{\partial x} \right) H \]

Add Slip

\[ V_L = \alpha V_g \]

Set 2 and 4 equal to each other and add slip

\[ \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \alpha \left[ \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{c_g}{\mu_g} H \right] \]
Insert Eqn 8 into 9 and solve for $c_L$

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \left[ \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) \right] H^2 + \frac{H}{\mu_g} \left[ \left( \frac{\partial p}{\partial x} \right) h + c_L - \left( \frac{\partial p}{\partial x} \right) H \right] \alpha
\]

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \alpha \left( \frac{\partial p}{\partial x} \right) H^2 + \frac{\alpha H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{\alpha H}{\mu_g} c_L - \frac{\alpha H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) H
\]

\[
\frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 + \frac{c_L}{\mu_L} h = \alpha^2 \left( \frac{\partial p}{\partial x} \right) + \frac{\alpha H}{\mu_g} \left( \frac{\partial p}{\partial x} \right) h + \frac{\alpha H}{\mu_g} c_L - \frac{\alpha H^2}{\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

\[
\frac{h}{\mu_L} c_L - \frac{\alpha H}{\mu_g} c_L = \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2
\]

\[
c_L \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right] = \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{2\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) + \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) h^2 - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

\[
c_L = \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)
\]

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Insert Eqn (7) into Eqn 8 and solve for \( c_g \)

\[
c_g = \left( \frac{\partial p}{\partial x} \right) h + \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H
\]

\[
c_g = \frac{\left( \frac{\partial p}{\partial x} \right) h \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]} + \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]
\]

\[
c_g = \frac{\left( \frac{\partial p}{\partial x} \right) h \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]} + \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]
\]

\[
c_g = \frac{\frac{h^2}{\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}
\]

\[
c_g = \frac{\frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{H h}{\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) - \left( \frac{\partial p}{\partial x} \right) H \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}
\]

\[
c_g = \frac{\frac{H h}{\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{h^2}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{\alpha H^2}{2\mu_g} \left( \frac{\partial p}{\partial x} \right)}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}
\]
The Liquid constant from equation 10 can be rewritten

\[ c_L = \frac{\alpha H h}{\mu_g} \left( \frac{\partial p}{\partial x} \right) - \frac{h^2}{2 \mu_L} \left( \frac{\partial p}{\partial x} \right) - \frac{\alpha H^2}{2 \mu_g} \left( \frac{\partial p}{\partial x} \right) = \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right] \left( \frac{\partial p}{\partial x} \right) = CC_L \left( \frac{\partial p}{\partial x} \right) \]

Where

\[ CC_L = \frac{\alpha H h}{\mu_g} - \frac{h^2}{2 \mu_L} - \frac{\alpha H^2}{2 \mu_g} \]

The Gas constant from equation 11 can be rewritten

\[ c_g = \frac{-H h}{\mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{h^2}{2 \mu_L} \left( \frac{\partial p}{\partial x} \right) + \frac{\alpha H^2}{2 \mu_g} \left( \frac{\partial p}{\partial x} \right) = \left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right] \left( \frac{\partial p}{\partial x} \right) = CC_g \left( \frac{\partial p}{\partial x} \right) \]

Where

\[ CC_g = \frac{-H h}{\mu_L} + \frac{h^2}{2 \mu_L} + \frac{\alpha H^2}{2 \mu_g} \]
Velocity Profiles from Equations 1 and 3 can be rewritten using DL and Dg.

The liquid velocity

\[ u_L = \frac{1}{2\mu_L} \left( \frac{\partial p}{\partial x} \right) y^2 + \frac{D_L}{\mu_L} \left( \frac{\partial p}{\partial x} \right) y \]

\[ u_L = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_L} y^2 + \frac{D_L}{\mu_L} y \right] \]

The gas velocity

\[ U_g = \frac{1}{2\mu_g} \left( \frac{\partial p}{\partial x} \right) Y^2 + \frac{D_g}{\mu_g} \left( \frac{\partial p}{\partial x} \right) Y \]

\[ U_g = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_g} Y^2 + \frac{D_g}{\mu_g} Y \right] \]
B.1.5 Liquid Volumetric Flow Rate

Now integrate velocity profile to attain volumetric flow rate.

\[ Q = \int_A \vec{V} \cdot d\vec{A} \]

For the liquid with channel width of \( a \)

\[ Q_L = \int_0^h u_L dy \]
\[ Q_L = \int_0^h u_L dy \]

\[ \frac{Q_L}{a} = \int_0^h \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_L} y^2 + \frac{CC_L}{\mu_L} y \right] dy \]

\[ \frac{Q_L}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L}{\mu_L} h^2 \right]_0 \]

\[ \frac{Q_L}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L}{\mu_L} h^2 \right] \]
B.1.6 Gas Volumetric Flow Rate

Now integrate velocity profile to attain volumetric flow rate.

\[ Q = \int_{A} \vec{V} \cdot d\vec{A} \]

For the gas with channel width of \( a \)

\[ Q_g = \int_{0}^{H} U_g adY \]

\[ \frac{Q_g}{a} = \int_{0}^{H} U_g dY \]

\[ \frac{Q_g}{a} = \int_{0}^{H} \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{2\mu_g} Y^2 + \frac{CC_g}{\mu_g} Y \right] dY \]

\[ \frac{Q_g}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_g} Y^3 + \frac{CC_g}{2\mu_g} Y^2 \right]_{0}^{H} \]

\[ \frac{Q_g}{a} = \left( \frac{\partial p}{\partial x} \right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g}{2\mu_g} H^2 \right] \]
B.1.7 Summary

The Liquid Volumetric Flow Rate is given by

$$\frac{Q_L}{a} = \left(\frac{\partial p}{\partial x}\right) \left[ \frac{1}{6\mu_L} h^3 + \frac{CC_L h^2}{2\mu_L} \right]$$

Where

$$CC_L = \frac{\frac{\alpha H h}{\mu_L} - \frac{h^2}{2\mu_L} - \frac{\alpha H^2}{2\mu_g}}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}$$

The Gas Volumetric Flow Rate is given by:

$$\frac{Q_g}{a} = \left(\frac{\partial p}{\partial x}\right) \left[ \frac{1}{6\mu_g} H^3 + \frac{CC_g H^2}{2\mu_g} \right]$$

Where

$$CC_g = \frac{\frac{H h}{\mu_L} + \frac{h^2}{2\mu_L} + \frac{\alpha H^2}{2\mu_g}}{\left[ \frac{h}{\mu_L} - \frac{\alpha H}{\mu_g} \right]}$$