A DETAILED REVIEW OF THE HEAT EXTRACTION METHOD
FOR THE MEASUREMENT OF LAMINAR FLAME SPEEDS

by

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ABSTRACT

The heat extraction method for measuring the laminar flame speed of a mixture is reviewed in detail. Great care is taken to minimize and document all sources of experimental uncertainty, and a detailed error analysis is presented. A simple one dimensional heat transfer model is developed to investigate the flow of heat through the system, and to apply a correction to the measured heat loss from the flame. This correction shifts the final value of laminar flame speed by as much as 20% of the flame speed uncertainty, or roughly 0.5 cm/s. Although other sources of uncertainty need to be addressed to decrease the size of the error bars, this shows that it is worth while to further investigate the heat flow through the flat flame burner. The experimental data is compared to literature data, as well as data simulated using the adiabatic freely propagating flame code, and the burner stabilized flame code, with GRIMech 3.0 as the reaction mechanism. Possible explanations are offered for variations in flame speed values amongst the different research groups, and their various measurement techniques. Additionally, deviations between the flame simulations and the experimental results are discussed. Possible plans are discussed for future work that could greatly improve this area of combustion research.
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CHAPTER 1

INTRODUCTION

Laminar flame speed has been the subject of many studies. It is a very important parameter because it offers some fundamental information about the mixture and the chemistry of its combustion reactions. Laminar flame speed is difficult to measure, because it is nearly impossible to establish a truly strainless, adiabatic, laminar flame in laboratory conditions. Thus, approximations must be made in order to measure laminar flame speed. Numerous techniques have been employed over the years to measure this parameter, each with its own set of assumptions and approximations.

The Spalding method, also known as the heat extraction method, is a very easy method to perform. The method uses a water cooled flat flame burner to measure the burner averaged flame speed, as well as the heat transferred from the flame to the burner, over a range of unburned gas flow rates. A plot is then made of burner averaged flame speed vs. flame heat loss, and the curve is extrapolated to zero heat loss to find the laminar flame speed. This method assumes that all of the heat loss from the flame goes to the cooling water. The primary focus of this thesis is to evaluate the validity of this assumption, as well as to investigate and minimize all other sources of experimental uncertainty. This will help researchers to determine whether the accuracy of this method meets their needs, or if another method should be investigated. To accomplish this, the heat extraction method was performed on methane-air flames, across a wide range of equivalence ratio. Methane-air was chosen because it is perhaps the most well documented combustible mixture, especially in terms of flame speed measurement. Additionally, there are several well established and validated chemical kinetic mechanisms and computer simulations that will provide simulated flame speed data to compare with experimental results. The wealth of data available on this mixture will make it much easier to evaluate the accuracy of this measurement technique.
Chapter 2 gives a brief overview of laminar flame theory, followed by a short review of several common laminar flame measurement techniques. Next, Chapter 3 gives a detailed experimental procedure for measuring laminar flame speed using the heat extraction method. A simple heat transfer model is developed to investigate the heat flowing through the burner, and a detailed error analysis is performed. In Chapter 4, the experimental data is compared to data from literature, as well as data from numerical flame simulations. Possible explanations are given for deviation between the various data sets. Finally, Chapter 5 offers some final conclusions, as well as suggestions for future work that would further this area of combustion research.
2.1 Laminar Flame Theory

A laminar flame is a deflagration wave that propagates through a flammable mixture of fuel and oxidizer. At ambient temperature and pressure, the mixture is essentially unreactive. For a flame to propagate through the mixture, an ignition source is needed. The source must provide enough energy to a local region of the mixture to bring it within the explosion limits. The resulting rapid reaction generates enough heat and radicals to bring the mixture in the surrounding region within its explosion limits, causing it to react as well. This chain reaction is the fundamental process behind the propagation of a laminar flame. The main objective in laminar flame theory is to determine the speed at which a deflagration wave will propagate through a given mixture. This parameter, $S_L$, is called the laminar flame speed, and is sometimes also referred to as adiabatic flame speed, or burning velocity. It is defined as the velocity of the unburned gas, relative and normal to the combustion wave surface. Laminar flame theory has been studied and developed by many researchers, attacking the problem from different angles. Based upon the assumptions made in developing each theory, the studies can be placed into the categories of thermal theory, diffusive-thermal theory, and detailed numerical simulation. The following discussion of flame theory follows the development in the books written by Glassman [1] and Kuo [2].
2.1.1 Thermal Theory

Mallard and Le Chatlier proposed that a flame is divided into two zones: the preheat zone and the reaction zone. In the preheat zone, the unburned gas is heated by conduction until it reaches the ignition temperature at the boundary between the two zones. The chemical reaction zone is where the reaction takes place and all of the heat is released. Their theory is based upon energy balance between the two zones:

\[ \dot{m} C_p (T_i - T_o) = \lambda \frac{T_f - T_i}{\delta_r} \] (2.1)

where the left side of the equation represents the energy absorbed in the preheat zone, and the right side represents heat flux into the preheat zone at the zone boundary. \( T_i \) is the ignition temperature, \( T_o \) is the unburned gas temperature, \( T_f \) is the flame temperature, \( \lambda \) is the thermal conductivity of the gas, and \( \delta_r \) is the thickness of the reaction zone. We know that \( \dot{m} \), the mass flow rate, is equal to the velocity of the unburned gas times its density. Assuming a flat plane flame, the velocity of the unburned gas is equal to \( S_L \), the laminar flame speed.

\[ \dot{m} = \rho S_L \] (2.2)

Combining equations 1 and 2 gives us:

\[ S_L = \frac{\lambda}{\rho C_p} \left( \frac{T_f - T_i}{T_i - T_o} \right) \frac{1}{\delta_r} \] (2.3)

We can also express the reaction zone thickness as \( \delta_r = S_L \tau_r \), where \( \tau_r \) is the reaction time. Since \( \tau_r \) is inversely proportional to \( RR \), the reaction rate, we can then write:

\[ \delta_r \propto S_L \frac{1}{RR} \] (2.4)

Combining equations 3 and 4 gives us:

\[ S_L \propto \sqrt{\alpha \cdot RR} \] (2.5)
where $\alpha$ is the thermal diffusivity. This is a very important result in laminar flame theory, because it is useful in estimating the effects of altering the physical and chemical properties of a combustion system. It should be noted that this theory assumes that $C_p$ and $\lambda$ remain constant across the flame. Also, the theory assumes that the temperature profile in the reaction zone is linear, and that its slope can be approximated as $(T_f - T_i)/\delta_r$. This development falls into the category of thermal theory because it considers only the transfer of heat, and does not take into account diffusion and the species conservation equations.

2.1.2 Diffusive-Thermal Theory

The theory of Mallard and Le Chatlier was improved by the Russian scientists, Zeldovich, Frank-Kamenetski, and Semenov. They combined the thermal theory of Mallard and Le Chatlier with the species conservation equations to develop a theory that includes diffusion of species as well as heat. However, they followed the insight of Mallard and Le Chatlier, that flame propagation is fundamentally a thermal mechanism, so they did not take into account the diffusion of radicals and its effect on the reaction rate. Instead, they were merely concerned with the energy transported by the diffusion of molecules. In developing this theory, several important assumptions were made:

1. Pressure is constant across the flame.

2. $C_p$ and $\lambda$ are constant.

3. $\lambda/C_p = D\rho$, where $D$ is the binary diffusion coefficient. Since we know that the Lewis number, $Le = \frac{\lambda}{\rho C_p D}$, it follows that $Le = 1$. This assumption gives the advantage of replacing one of the differential equations with an algebraic equation.

4. Finally, the flame is assumed to be a one dimensional, steady state flame.
These assumptions are used when applying the energy and mass balance equations across a differential control volume that represents the flame. Figure 2.1 shows the energy and mass balance equations used to describe the flame.

\[
\begin{align*}
T & \rightarrow \quad \rightarrow T + \frac{dT}{dx} \Delta x \\
\dot{m} C_p T & \rightarrow \quad \rightarrow \dot{m} C_p (T + \frac{dT}{dx} \Delta x) \\
-\lambda \frac{dT}{dx} & \rightarrow \quad \rightarrow -\lambda \frac{dT}{dx} (T + \frac{dT}{dx} \Delta x) \\
a/\rho & \rightarrow \quad \rightarrow a/\rho + \frac{d(a/\rho)}{dx} \Delta x \\
-D \rho \frac{d(a/\rho)}{dx} & \rightarrow \quad \rightarrow -D \rho \frac{dx}{dx} \left(\frac{a}{\rho} + \frac{d(a/\rho)}{dx} \Delta x\right)
\end{align*}
\]

Figure 2.1. Balances Across a Differential Element Describing a Laminar Flame

Applying boundary conditions and solving, yields the following expression for flame speed:

\[
S_L = \sqrt{2 \left( \frac{\lambda}{\rho C_p} \right) \frac{I}{T_f - T_o}}
\]

(2.6)

where

\[
I = \frac{1}{a_o} \int_{T_i}^{T_f} \dot{\omega} \, dT
\]

(2.7)

and

\[
\dot{\omega} = A \, e^{-E/RT}
\]

(2.8)

Equation 2.8 is the Arrhenius expression, where A is the pre exponential constant, \(E_a\) is the activation energy of the reaction, and R is the ideal gas constant. For mixtures with high activation energy, such as hydrocarbon-air mixtures, most of the reaction
occurs near the flame temperature, so the integral can then be approximated as:

\[ I = \frac{1}{a_o} \int_{T_o}^{T_f} \dot{\omega} \, dT \]  \hspace{1cm} (2.9)

This is a huge advantage because it eliminates the ignition temperature, \( T_i \), which is unknown. Since no reaction takes place at \( T_o \), the integral can then be evaluated and written as:

\[ I = \frac{A \, RT_f^2}{a_o \, E} \, e^{-E/RT_f} \]  \hspace{1cm} (2.10)

The expression for flame speed then becomes:

\[ S_L = \sqrt{2 \left( \frac{\lambda}{\rho c_p} \right) \frac{1}{a_o} \left( A \, e^{-E/RT_f} \right) \frac{RT_f^2}{E(T_f - T_o)}} \]  \hspace{1cm} (2.11)

This is a very important result because it relates flame speed directly to the physical properties of the unburned mixture, as well as the reaction rate of the mixture.

### 2.1.3 Detailed Numerical Simulation

Using computers, it is possible to develop numerical techniques to solve the comprehensive mass, species, and energy conservation equations. For simulation of laminar premixed flames, the most widely used code is the freely propagating flame code developed by Kee et al. [3]. It simulates a one dimensional, adiabatic, freely propagating, premixed flame. The user supplies a complete reaction mechanism, thermodynamic properties, and transport properties of all species in the mechanism. The code then uses a hybrid time-integration/Newton-iteration technique to solve the flame equations. It then returns all of the information about the flame, including species profiles, temperature profiles, flame speed, and all of the gas properties throughout the flame.

The majority of the work done in comprehensive theory focuses on developing
the reaction mechanism, thermodynamic data, and transport properties to be used as input for the flame code. The most widely used mechanism is GRIMech [4]. It has been optimized for simulation of methane-air flames, and is widely recognized as the best available mechanism for methane-air combustion. Creation and optimization of a mechanism is a long and difficult process. It begins by starting with a complete set of elementary reactions, and assigning a reaction rate constant to each reaction. Next, literature is searched for reliable experiments that are relevant to the combustion system being modeled by the mechanism. This includes various shock tube experiments, flame measurements, ignition studies, and flow reactor studies that depend on some or all of the rate and transport parameters in the model. The model is then solved and the output is compared to all relevant experimental data. Next, the rate constants and transport properties are adjusted within their appropriate uncertainties, and the model is solved again. This lengthy process is repeated until the best possible fit to experimental data is obtained. When creating a new reaction mechanism, researchers often start with an existing mechanism, and then modify it to fit the combustion system that they are studying.

2.2 Laminar Flame Speed Measurement

Laminar flame speed has been measured by many different experimentalists, using many different methods. The ideal method of flame speed measurement would involve the establishment of an adiabatic, strainless flame, that is controllable over a wide range of conditions. This ideal method does not exist. Experimentalists have not agreed upon a single standard method because it is nearly impossible to establish a flame that is both adiabatic and strainless in laboratory conditions. Thus, approximations must be made when measuring flame speed. Due to the large variety of measurement techniques, and their associated approximations, published flame speed data for a given mixture can have a wide range of values. As discussed in the review of flame speed measurements by Andrews and Bradley [5], the various methods of measuring flame speed can be placed into two main categories: stationary flames and non stationary flames. In stationary flames, the flame is fixed in the laboratory reference frame, and unburned gas moves through the fixed combustion wave. An example is
a Bunsen burner, where the flame is stabilized at the opening of the burner. In non stationary flames, the flame propagates through the initially stationary gas mixture. An example is the tube method, in which a tube filled with gas is ignited at one end, and the flame propagates through the tube. I will now examine and compare some of the common methods of measuring flame speed.

2.2.1 Non Stationary Flames

Tube Method

The tube method involves filling a tube with the gas mixture, lighting it at the open end, and measuring how fast the flame propagates through the tube. However, the pressure wave created by the expansion of the burning gas changes the density and velocity of the unburned gas. The mass conservation equations can be used to derive a theoretical expression for the adiabatic flame speed in terms of the measured speed of propagation. In deriving this expression, it is assumed that the flame speed is constant over the cross section of the tube, and that the surface area of the flame is constant. However, the flame aerodynamics change as the flame propagates, distorting its shape. Additionally, the walls of the tube absorb some of the heat produced by the flame. This causes the flame to propagate slightly slower near the walls, further distorting its shape and altering the overall rate of propagation. The assumptions made in deriving the expression for adiabatic flame speed are therefore not entirely valid, and may be significant sources of error [5].

Contained Explosions

The most common of the contained explosion methods is the spherical constant volume bomb. In this method, a spherical vessel is filled with the gas mixture, which is
then ignited at the center. The result is a spherical combustion wave that propagates radially outward inside the vessel. To determine the flame speed, one must measure $dr/dt$ vs. time, as well as vessel pressure vs. time. Using conservation of mass, an expression can be written for the adiabatic flame speed in terms of $dr/dt$ and the vessel pressure. For a complete derivation and discussion of the procedure, see Manton et al. [6]. This method can be very accurate if done properly, but it requires a complicated apparatus. It can be difficult to accurately measure the combustion wave velocity vs. time, as well as the vessel pressure vs. time.

Andrews and Bradley [7] used a variation of the constant volume bomb technique, called the double kernel method. In this method, two flames are simultaneously ignited inside the chamber. The gas velocity halfway between the flames is zero. Therefore, the adiabatic flame speed is the velocity of each of the flame kernels, right as they meet in the middle. The explosions were filmed using schlieren imaging with a high speed rotating prism camera. The biggest complication in this method is getting the flames to ignite simultaneously. Andrews and Bradley were only able to get the flames to ignite within a few milliseconds of each other. This allows the first flame to propagate as much as .5 cm before the second flame is ignited. Another complication is that the flames sometimes propagate obliquely to the optical path. When this happens, the high speed film shows the flames meeting, when in fact, a large distance still remains between them. These complications result in flame speed measurements that are too high.

2.2.2 Stationary Flames

Bunsen Burner

The Bunsen burner is perhaps the simplest method of measuring flame speed. A premixed flame is established at the end of the burner tube, and the flame speed is calculated simply by dividing the volume flow rate of the unburned gas by the area of
the flame. However, the Bunsen burner flame is neither adiabatic, nor strainless. The flame speed is slower at the edges near the tube walls where there is heat loss, and faster near the tip where the flame is strained. Therefore, dividing the by the flame area gives an average flame speed over the flame surface and does not necessarily give an accurate measure of the adiabatic flame speed of the mixture. The simplicity of this method makes it an excellent way to get a ballpark estimate of the flame speed, but compared to other methods, it is not very accurate [5].

**Premixed Counter Flow Twin Flames**

The premixed counter flow twin flames method was developed by C. K. Wu and C. K. Law [8]. The method involves creating a counter flow by impinging two identical premixed jets, creating a stagnation plane in the center. Then the counter flow is ignited, and two identical flames are established, one on each side of the stagnation plane. The flame speed can then be measured by laser doppler velocimetry, or another particle tracking technique. The flame speed is simply the velocity of the gas just prior to the combustion zone. This method has the advantage that the flames are essentially adiabatic because, except for radiative heat loss, all of the heat generated in the combustion goes towards heating up the unburned gas. However, this alone does not provide the adiabatic flame speed, because the flames are strained. To determine the laminar flame speed, the strained flame speed must be measured over a range of flame strain rates. The plot of flame speed vs. strain rate can be extrapolated to zero strain rate, providing a value for the adiabatic flame speed. This is arguably the most accurate method for measuring adiabatic flame speed. However, relative to other methods, it is a much more difficult experiment to set up.

**Stagnation Plane Method**

The stagnation plane method was developed by C. M. Vagelopoulos and F. N. Egolfopoulos [9]. It involves establishing a premixed flame in a stagnation flow confi-
ration, with a large separation distance between the jet nozzle and the steel plate used as the stagnation plane. The large separation distance allows for the establishment of planar flames at higher flow rates, and Bunsen-type flames at lower flow rates. The technique relies on the fact that the planar flames have a positive strain rate, while the Bunsen-type flames have a negative strain rate. A planar flame is established, and then the flow rate is gradually decreased, and the flame makes a steady, smooth transition to a Bunsen-type flame. As the flame makes this transition, it passes through a near-zero strain rate state. The flow velocity is measured in real-time using laser doppler velocimetry, and the laminar flame speed is equal to the flow velocity just as the flame transitions through the zero-strain state. This method has the advantage that the laminar flame speed is directly measured, and no extrapolation is required. However, just like the counter flow method, this is a more complicated experiment to perform.

**Flat Flame Methods**

Flat flame burners usually have a cylindrical burner surface, consisting of a porous plug or an array of tubes. This serves to direct the unburned gas into a uniform flow field that is perpendicular to the burner surface. Flat flame methods are similar to the Bunsen burner method because the flame speed is usually determined by dividing the volume flow rate of the gas by the area of the flame. However, this is sometimes accompanied by a particle tracking technique for added accuracy. Also, like Bunsen burner flames, flat flames are non adiabatic because there is heat loss to the burner surface. The advantage of flat flames lies in the fact that they are essentially strainless, because the flame is established in the uniform flow field above the burner surface. Because of this, heat loss is the only thing that must be accounted for in order to determine the adiabatic flame speed. There are two methods commonly used to account for the heat loss and determine the adiabatic flame speed.

The heat flux method was first described by VanMaaren et al. [10], and a detailed analysis of the method is provided by Bosschaart et al. [11]. The method uses ther-
mocouples to measure the radial temperature gradient of the burner, which is used to calculate the rate of heat transfer from the flame to the burner. The burner is surrounded by a water jacket that is used to heat the edges of the burner. The water temperature and flow rate is adjusted until the temperature gradient on the burner surface is very small. The result is essentially an adiabatic flame, because the heat lost to the burner is replaced by the water heating the unburned gas.

The next method, and the focus of this study, is the Spalding method, also known as the heat extraction method. As described in Chapter 1, this flat flame technique involves measuring the flame speed and the heat transfer from the flame to the burner, across a range of gas flow rates. A plot is then made of flame speed vs. heat loss, and the adiabatic flame speed is determined by extrapolating to zero heat loss. Botha and Spalding measured the heat loss of the flame by cooling the burner with a water tube coiled around the sides of the burner cylinder. The heat loss is calculated by measuring the mass flow rate of the water, and the temperature increase of the water after it has passed through the cooling tube [12].
CHAPTER 3

EXPERIMENT

3.1 Heat Extraction Method

The experiment is started by establishing a flame with a high flow rate such that the flame stands off from the burner. After the burner reaches equilibrium, flame speed and heat loss are measured. Next, the flow rate is decreased while keeping the equivalence ratio constant, and the measurements are taken again. The lower flow rate brings the flame closer to the burner, increasing the heat loss from the flame, and slowing its flame speed. This process is repeated until the flow rate is too low to support a flame, or the lower limit of the mass flow controllers is reached. Then, the equivalence ratio is switched and the experiment is started over.

This is slightly different than the procedure used by Spalding and Botha, who published their paper in 1954. Without the availability of modern mass flow controllers, they had to control the flow rates of their gas using needle valves, while constantly measuring the flow rate using glass capillary flow meters and manometers. Starting with a very rich, semi-diffusion flame, they held the oxidizer flow constant, while decreasing the fuel flow rate after each measurement. This was repeated until the lean flammability limit was reached and the flame extinguished. Next, the oxidizer flow rate was lowered slightly, the fuel was turned back up, and the procedure was started again with a new rich flame [12]. Spalding and Botha likely designed the procedure this way because it was more efficient for them to only adjust one gas flow rate for each data point. Today, mass flow controllers can quickly and accurately adjust gas flow rates simply by inputting a control voltage in a computer. Thus, it is now equally practical to adjust the fuel and oxidizer at the same time, holding equivalence
ratio constant. Both procedures yield identical results, as long as enough time is given for the burner to reach equilibrium at each flow rate before the measurements are recorded. This is convenient because it is often desirable to measure the adiabatic flame speed of a single mixture ratio.

3.1.1 Apparatus

Figure 3.2 shows a diagram of the flat flame burner used to carry out the experiments. The burner was designed and built by McKenna Products, Inc., now called Holthius and Associates [13]. The burner surface is 6 cm in diameter, and is constructed of a sintered porous bronze plug. The burner is water cooled, using a coil of copper tubing which is embedded in the burner plug. This serves to keep the burner nearly isothermal in the radial direction, while the heat is all pulled out in the axial direction. This is different than the burner used by Spalding and Botha, which was cooled by a tube coiled around the sides of the burner. This causes a temperature gradient across the burner surface in the radial direction, which affects the uniformity of the flame.

The burner plug is surrounded by a sintered porous ring, used to introduce an inert shroud gas flow that is coaxial with the flow of the unburned gas. This is all assembled into a stainless steel burner housing, which includes the connections for cooling water, reactant gases, and the inert shroud gas. The inlet and outlet temperatures of the cooling water were measured using K-type thermocouples, that were fully submerged in the water stream. The cooling water pressure was adjusted using a needle valve pressure regulator, and the flow rate was measured using a graduated cylinder and a stopwatch. The gas flow was regulated using mass flow controllers (MFCs) built by Teledyne Hastings Instruments. The MFCs were controlled using a LabView VI that was written by Micah Jakulewicz [14]. The VI is a simple PID controller that allows the user to input the desired voltage and displays the voltage returned by the MFCs. The MFCs were calibrated using a Bios International Dry Cal flow meter (DC2).
3.1.2 Detailed Procedure

First, the freely propagating flame simulation in Cantera is used to get an estimate of the adiabatic flame speed of the mixture [15]. A series of measurements is then started by igniting a flame with a gas flow rate such that the velocity of the unburned gas as it exits the burner is roughly 25% faster than the adiabatic flame speed of the mixture. The result is a flame that is pushed away from the burner surface. It is also very wrinkled, giving it a high enough surface area to avoid being blown off. If a flame simulation is not available to estimate the adiabatic flame speed, then trial and error can be used to establish an initial flame that stands off from the burner. The flow of the nitrogen shroud gas is set so that the momentum of the nitrogen matches the momentum of the unburned mixture. The system is given time to reach equilibrium, and then the inlet and outlet water temperatures are recorded. While waiting for the system to reach equilibrium, the flow rate of the cooling water is checked because the supply pressure varies with building water usage. If the water flow rate has deviated from its original value, it is adjusted accordingly.
Next, the gas flow rate is decreased by 10%, while holding the mixture equivalence ratio constant. This brings the flame a little closer to the burner, and makes it a little less wrinkled. The cooling water flow rate is again checked while the system is allowed to reach equilibrium, and then the temperatures are recorded. The procedure is repeated until the MFCs reach their lower limit, or until the flow rate becomes too low and the flame is quenched by the burner surface.

After the gas flow rate has been decreased three times, the exit velocity of the unburned gas drops below the adiabatic flame speed of the mixture. Theoretically, when this happens, the flame will no longer be wrinkled; it will become flat and attached to the burner surface. In practice, however, the heat loss to the burner slows down the reaction rate and flame speed. As a result, the flame does not become flat and attached to the burner surface until the exit velocity of the unburned gas has dropped to roughly 85% of the adiabatic flame speed. It is important to note which data point comes from measurements of the first attached flat flame, because this is the first data point that will be used in the linear extrapolation to the adiabatic flame speed.

The next step is to plot the average flame speed (m/s) vs. the heat loss of the flame (Joules/mL fuel). The average flame speed can be determined by taking the volume flow of the unburned gas (referenced to laboratory temperature and pressure) and dividing it by the area of the burner surface. As described earlier, the heat loss is calculated from the temperature rise and flow rate of the cooling water. It is expressed in units of Joules/ml fuel in order to provide the linear region for extrapolation to adiabatic flame speed. Decreasing the flow rate causes the flame to move closer to the burner, increasing the heat transfer to the burner. As the flow is decreased, a maximum amount of heat transfer is quickly reached. Further decreasing the flow only decreases the amount of heat generated by the flame and starts to bring it towards extinction. This causes the curve of flame speed vs heat loss to be nonlinear. Dividing the rate of heat transfer by the volume flow rate of the fuel is a way of normalizing the data by the amount of energy available in the reaction. The weak flames with less heat transfer have a smaller methane flow rate, so the heat loss value gets divided by a smaller number than the hotter flames. The result is a linear region that can easily
be extrapolated to zero heat loss, providing the value of the adiabatic flame speed.

3.2 Simple Heat Transfer Model

Development of a simple heat transfer model can greatly expand our understanding of the heat flow through the burner. The heat extraction method assumes that all of the heat transferred from the flame to the burner is carried away by the cooling water. A simple model can be used to examine this assumption, and explore other mechanisms through which heat may flow from the burner. Additionally, an objective of this study is to compare the experimental results with the burner stabilized flame model in Chemkin and/or Cantera. These flame simulations require the user to input the burner surface temperature. The way that the McKenna burner is designed makes it difficult to directly measure the burner surface temperature without disturbing the flame. Also, the attached flames sit so close to the burner surface that the temperature measurement device would be heated by the flame, resulting in a temperature reading that is higher than the actual burner surface temperature. With a simple heat transfer model, the burner surface temperature can be estimated, enabling a comparison to the burner stabilized flame simulation.

3.2.1 Burner Head

The burner surface temperature, as well as the exit temperature of the unburned gas, can be estimated using a one dimensional heat transfer model. Given the cylindrical burner geometry, the model can be made to be one dimensional by making the following assumptions:

1. The thermal conductivity of the porous plug is high enough that the plug can be considered to be isothermal in the radial direction. All temperature gradients and heat transfer then occur in the axial direction only.
2. The heat transfer between the unburned gas and the porous plug occurs so rapidly that the gas is nearly in thermal equilibrium with the plug at all points of the flow. Thus, the exit temperature of the gas can be approximated as being equal to the temperature of the burner surface. This assumption can be rationalized by the fact that the amount of energy it takes to heat the gas is less than 2% of the energy that is being conducted through the burner to the water.

The first step is to derive an expression for the average temperature of the cooling tube coil, \( T_T \), in terms of the inlet and outlet temperatures of the cooling water, \( T_{H_2O,in} \) and \( T_{H_2O,out} \). This can be done by using the internal flow relations from Chapter 8 in Incropera and DeWitt [16]. The relation is chosen by calculating the Reynolds number and the Prandtl number of the water flow through the cooling tube. For the cooling tube and water flow rate, the flow is laminar, and the Prandtl number is greater than 0.6. For this flow situation, there are two relations that can be used. One assumes constant heat flux, and the other assumes constant tube temperature. Since we are assuming that the burner is isothermal in the radial direction, we will assume that the same is true of the cooling tube coil, so we will choose the uniform temperature relation:

\[
Nu_D = 3.66 = \frac{\bar{h}D}{k_{H_2O}} \quad (3.1)
\]

\[
\bar{h} = \frac{\dot{m}C_{p,H_2O} \left( T_{H_2O,out} - T_{H_2O,in} \right)}{\pi DL} \frac{\Delta T_{im}}{\Delta T_{im}} \quad (3.2)
\]

\[
\Delta T_{im} = \frac{T_{H_2O,in} - T_{H_2O,out}}{\ln \left[ \frac{T_T - T_{H_2O,out}}{T_T - T_{H_2O,in}} \right]} \quad (3.3)
\]
By combining Equations 3.1, 3.2, and 3.3, we can then solve for the average temperature of the cooling tube:

\[ T_T = \frac{T_{H_2O,\text{out}} - T_{H_2O,\text{in}} \exp \left( \frac{-3.65 \pi k_{H_2O} L}{m_{c_p,H_2O}} \right)}{1 - \exp \left( \frac{-3.65 \pi k_{H_2O} L}{m_{c_p,H_2O}} \right)} \]  

(3.4)

Next, the temperature of the burner surface, \( T_s \), can be solved for by writing the energy balance across the burner plug. In order to write the energy balance equations, the burner plug will be examined in three separate regions. Region 1 is the portion of the porous plug that is behind the cooling tube coil. Region 2 extends from the cooling tube to the burner surface. The final region is the cooling tube itself. Figure 3.2 illustrates the heat flow through this system.

![Figure 3.2. Burner Energy Balance](image-url)

Figure 3.2. Burner Energy Balance
The energy balance across Region 2 can be written as follows:

$$\dot{q}_f = (\dot{q}_{\text{gas},T_s} - \dot{q}_{\text{gas},T_T}) + \dot{q}_T$$  \hspace{1cm} (3.5)$$

where $\dot{q}_f$ is the rate of heat transfer from the flame to the burner, $\dot{q}_T$ is the rate of heat conduction from Region 2 into the tube region, and $(\dot{q}_{\text{gas},T_s} - \dot{q}_{\text{gas},T_T})$ represents the power consumed in heating the gas as it flows through Region 2. Next, write the energy balance across the tube region:

$$\dot{q}_T = \dot{q}_{H_2O} + \dot{q}_1 + \dot{q}_{\text{gas},T_T} - \dot{q}_{\text{gas},T_1}$$  \hspace{1cm} (3.6)$$

where $\dot{q}_1$ is the rate of heat conduction into Region 1. The heat transfer rate to the cooling water, $\dot{q}_{H_2O}$, can be written as:

$$\dot{q}_{H_2O} = \dot{m}_{H_2O} C_{pH_2O} (T_{H_2O,\text{in}} - T_{H_2O,\text{out}})$$  \hspace{1cm} (3.7)$$

Since $T_T$ is equal to $T_1$, Equation 3.6 can be rewritten as:

$$\dot{q}_T = \dot{q}_{H_2O} + \dot{q}_1$$  \hspace{1cm} (3.8)$$

The heat conducted into Region 1 is consumed entirely in heating the unburned gas from laboratory temperature, $T_{\text{Lab}}$, to the temperature of the cooling tube, $T_T$. Energy balance across Region 1 then gives us:

$$\dot{q}_1 = \dot{q}_{\text{gas},T_1} - \dot{q}_{\text{gas},T_{\text{Lab}}}$$
$$\dot{q}_1 = \dot{q}_{\text{gas},T_T} - \dot{q}_{\text{gas},T_{\text{Lab}}}$$  \hspace{1cm} (3.9)$$

Since $\dot{q}_T$ is the rate of energy conduction through Region 2 into the tube region, it can be rewritten as:

$$\dot{q}_T = k_b A_b \frac{(T_s - T_T)}{L} = \dot{q}_{H_2O} + \dot{q}_1$$  \hspace{1cm} (3.10)$$
where \( k_b \) is the thermal conductivity of the burner plug and \( A_b \) is the area of the burner surface. Combining Equations 3.9 and 3.10 then allows us to solve for \( T_s \):

\[
T_s = \left( \dot{q}_{H_2O} + \dot{q}_{gas,T_T} - \dot{q}_{gas,T_{Lah}} \right) \frac{L}{k_b A_b} + T_T
\]  

(3.11)

The exact composition and porosity of the burner plug are not known. The plug is constructed of a sintered bronze alloy. *Heat Transfer Handbook*, by Bejan and Krause, states that sintered copper based alloys typically range in porosity from 9-34% [17]. The book by J. B. Austin, *The Flow of Heat in Metals*, offers the following expression for relating porosity of sintered metals to their thermal conductivity:

\[
k_s = k_p \frac{1 - P}{1 + \frac{P}{2}}
\]  

(3.12)

where \( k_s \) and \( k_p \) are the thermal conductivity of the sintered and pure metal, respectively, and \( P \) is the porosity of the sintered metal [18]. This gives a range of thermal conductivity from 30 to 47 W/m²K. Assume that \( k_b \) is in the middle of this range. This makes the uncertainty in \( k_b \) equal to half the range, or 8.5 W/m²K. Based upon the amount of heat being conducted through the burner plug for the hottest stoichiometric flames, the uncertainty in \( k_b \) produces an uncertainty \( T_s \) of only 0.2 K.

With Equation 3.10, the burner surface temperature can be easily evaluated for each flame, using nothing more than the measurements already recorded while performing the experiment. From examining the energy balance of the system, it is clear that the amount of heat transferred from the flame to the burner is larger than that measured with the cooling water; some of the energy goes into heating the unburned gas from room temperature to \( T_s \). However, this energy will not be included in the total heat loss from the flame for the extrapolation. This is because it is ultimately brought back to the flame in the form of an elevated unburned gas temperature, working to increase the reaction rate and the flame speed. However, this is not the only method through which heat leaves the burner unaccounted for. In the next section, we will consider the heat that is conducted through the sides of the plug into the nitrogen shroud ring.
3.2.2 Heating of Nitrogen Shroud Gas

The heat transfer model presented in the previous section assumes that the burner is isothermal radially, with heat flowing only in the axial direction. This would mean that no heat is conducted out through the sides of the burner, and into the nitrogen shroud ring and burner housing. However, with a flame established, turning the nitrogen shroud gas on or off has an observable effect on the output temperature of the cooling water. This means that possibly a significant amount of heat is conducted out to the shroud ring, and is carried away by the shroud gas.

The rate at which heat is conducted into the nitrogen shroud ring can be estimated by observing the effect that the nitrogen flow has on the system. Consider the measurements from one of the flames used in the linear extrapolation for the stoichiometric flame speed. With this flame ignited and the nitrogen shroud gas flowing, the flame produced a temperature increase in the cooling water of 16.1 degrees C. This translates to 177 Joules/s carried away by the cooling water. Next, the nitrogen shroud gas was shut off, and the system was allowed to return to equilibrium. This caused the output water temperature to rise by an additional 0.3 degrees C. This translates to an additional 3.3 Joules/s transferred to the water as a result of shutting off the nitrogen gas flow. This is likely a good estimate for the rate that heat is carried away by the nitrogen shroud gas for this flame. For comparison, this is roughly 2% of the rate that heat energy is extracted by the water.

The shroud ring is made of the same sintered material as the burner plug. Therefore, we will make the same assumption that was made in the burner head heat transfer model; the heat transfer from the sintered metal of the shroud ring to the nitrogen happens so rapidly that the nitrogen is in equilibrium with the ring as it exits. Since there is a thin stainless steel wall between the burner plug and the nitrogen shroud ring, the exit temperature of the nitrogen gas must be lower than the burner surface temperature. For comparison, Table 3.1 shows the rate of heat transfer necessary to heat the nitrogen shroud gas to various different temperatures. The lowest temperature is $T_t$, the cooling tube temperature. The highest is $T_s$, the burner surface temperature. The middle temperature is $T_{ts,ave}$, the average between $T_t$ and $T_s$. 
Table 3.1. Power to Heat the Nitrogen Shroud Gas to $T_{Exit}$ for $\dot{V}_{N_2} = 7.9$ SLM

<table>
<thead>
<tr>
<th>N$<em>2$ Exit Temperature ($T</em>{Exit}$)</th>
<th>Heat Transfer (Watts)</th>
</tr>
</thead>
<tbody>
<tr>
<td>309.5 K</td>
<td>2.6</td>
</tr>
<tr>
<td>313.75 K</td>
<td>3.3</td>
</tr>
<tr>
<td>318 K</td>
<td>4</td>
</tr>
</tbody>
</table>

For this flame, the rate of heat transfer required to heat the nitrogen to $T_{tS,ave}$ is the same as the increase in heat transfer to the water when the nitrogen is shut off. This suggests that $T_{tS,ave}$ is a fairly good estimate of $T_{Exit}$ of the nitrogen shroud gas. Assume that for every flame, the nitrogen shroud gas is heated to $T_{tS,ave}$. We can then calculate the rate of heat transfer to the nitrogen gas for every flame, and add it as a correction to the values of flame heat loss.

Figure 3.3 shows the experimental data for the stoichiometric flames, both with and without the heat transfer to the nitrogen. Figure 3.4 shows the same curves for the $\Phi = 1.6$ data. The uncorrected data is shown only by the intersection of its vertical and horizontal error bars. The corrected data points are displayed as square symbols. As shown in Figure 3.3, the nitrogen correction shifts the $\Phi = 1$ data points
Figure 3.4. Effect of the $N_2$ Shroud Correction on the $\Phi = 1.6$ Data

horizontally by as much as 75% of the error bars. Also shown, are the linear fit lines for both the uncorrected and the corrected data, and the significant shift created by the correction. As shown in Figure 3.4, the effect of the nitrogen correction on the $\Phi = 1.6$ data is very small. This is expected since the amount of heat generated by this flame is very small. The corrected data points are nearly directly on top of the uncorrected data points, and the linear extrapolations are almost identical. Using the Method of Least Squares for the extrapolation allows us to calculate the uncertainty of the final extrapolated value of adiabatic flame speed, $\sigma_{SL}$. For the $\Phi = 1$ data, the nitrogen correction shifts the final extrapolated adiabatic flame speed value by nearly 20% of $\sigma_{SL}$. It is therefore appropriate to include this correction in the $\Phi = 1$ data. As shown by the $\Phi = 1.6$ data, this shift is much smaller for the slower flames that generate smaller amounts of heat. However, the correction is easy to include, so it will be included in the analysis of every equivalence ratio. See Section 3.3 for a detailed error analysis.

We have determined that the effect of the nitrogen shroud heating is significant enough to be included in the experimental data. However, the exit temperature of the
nitrogen is a very rough estimate. In future studies, it would be beneficial to measure its exit temperature directly, or develop a more detailed, 3-D heat transfer model of the burner. This would give a more detailed look at the heat flow through the system, and better evaluate the different modes through which escapes.

3.3 Error Analysis

When using the heat extraction method, there are several places where experimental uncertainty is introduced. Uncertainty in the measured flame speed comes from the flow of gas through the mass flow controllers, the room temperature measurement, and the flame diameter. Uncertainty in the flame heat loss measurement comes from the water flow rate and water $\Delta T$ measurements. The flow rate of the methane also contributes to heat loss uncertainty since the heat loss is expressed in units of Joules/mL methane. Finally, uncertainty from the mass flow controllers also creates uncertainty in the equivalence ratio of the flames. Table 3.2 is a summary of the experimental measurements and their uncertainties.

Table 3.2. Uncertainties in Experimental Measurements

<table>
<thead>
<tr>
<th>Quantity Measured</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water flow rate</td>
<td>0.1 mL/s</td>
</tr>
<tr>
<td>Water $\Delta T$</td>
<td>0.2 K</td>
</tr>
<tr>
<td>Lab Temperature ($T_L$)</td>
<td>1.5 K</td>
</tr>
<tr>
<td>Lab Pressure ($P_L$)</td>
<td>.005 Atm</td>
</tr>
<tr>
<td>Gas Flow</td>
<td>1% MFC reading (SLM)</td>
</tr>
<tr>
<td>Burner Diameter ($d_b$)</td>
<td>0.2 mm</td>
</tr>
</tbody>
</table>

Now that the experimental uncertainties are known, we must determine how they propagate through the system and affect the measured values of flame speed, heat loss, and equivalence ratio.
3.3.1 Flame Speed Uncertainty

First, consider the uncertainties in the flame speed measurement. Equation 3.13 is the expression for flame speed in terms of the experimental parameters:

\[ S_{ave} = \frac{F_L}{A_b} \]

\[ = \frac{F_S T_L P_{stp}}{\pi \frac{a^2}{4} T_{stp} P_L} \]  

(3.13)

\( T_L \) and \( P_L \) are the laboratory temperature and pressure. \( T_{stp} \) and \( P_{stp} \) are the standard temperature and pressure, \( 273.15 \, \text{K} \) and one atmosphere, respectively. \( F_S \) is the gas flow rate in standard liters per minute (SLM) that is returned by the mass flow controllers. Equation 3.13 also shows the conversion factor required to calculate \( F_L \), the flow rate in L/min at laboratory temperature and pressure. The uncertainty of the mass flow controllers is determined by their calibration, which was performed using the Bios Dry-Cal II [19]. The calibration fits are good enough that the difference between each calibration point and the fit curve is an order of magnitude smaller than the calibrator uncertainty. Teledyne-Hastings does a factory calibration on the mass flow controllers, and specifies an uncertainty of 1% full scale. However, due to the high quality of the Dry-Cal II calibration fits, the mass flow controller uncertainty can be approximated as being equal to the calibrator uncertainty (±1% of reading). Following standard propagation of error technique, we can derive the following expression for the uncertainty in \( S_{ave} \):

\[ \sigma_{S_{ave}}^2 = \left( \frac{\delta S_{ave}}{\delta F_S} \sigma_{F_S} \right)^2 + \left( \frac{\delta S_{ave}}{\delta T_L} \sigma_{T_L} \right)^2 + \left( \frac{\delta S_{ave}}{\delta P_L} \sigma_{P_L} \right)^2 + \left( \frac{\delta S_{ave}}{\delta d_f} \sigma_{d_f} \right)^2 \]  

(3.14)

where \( \sigma_{F_S}, \sigma_{T_L}, \) and \( \sigma_{d_f} \) are the uncertainties in the parameters.
3.3.2 Heat Loss Uncertainty

The same technique will be used to find an expression for the uncertainty in the heat loss measurement. Begin with the expression for $\dot{q}_f$, the rate of heat loss to the burner:

$$\dot{q}_f = \frac{\dot{V}_{H_2O} \rho_{H_2O} C_{p_{H_2O}} \Delta T_{H_2O}}{F_{CH_4}}$$

(3.15)

where $\dot{V}_{H_2O}$ is the flow of cooling water in mL/s, $\rho_{H_2O}$ is the density of water, $C_{p_{H_2O}}$ is the specific heat of water, $\Delta T_{H_2O}$ is the temperature rise of the water after flowing through the burner, and $F_{CH_4}$ is the flow of methane in mL/s. The expression for uncertainty in $\dot{q}_f$ can be written as:

$$\sigma_{\dot{q}_f}^2 = \left(\frac{\delta \dot{q}_f}{\delta \dot{V}_{H_2O}} \sigma_{\dot{V}_{H_2O}}\right)^2 + \left(\frac{\delta \dot{q}_f}{\delta \Delta T_{H_2O}} \sigma_{\Delta T_{H_2O}}\right)^2 + \left(\frac{\delta \dot{q}_f}{\delta F_{CH_4}} \sigma_{F_{CH_4}}\right)^2$$

(3.16)

Now that we have expressions for the uncertainty in $S_{avo}$ and $\dot{q}_f$, we can perform a linear extrapolation to the adiabatic flame speed. For this, we will use the Method of Least Squares. The data points from the first several attached flames will be used in the extrapolation. The data points have both horizontal and vertical error bars. However, the Method of Least Squares only takes into account the vertical error bars. A fit is first made using just the vertical error bars. Then, the slope of this line is used to translate the horizontal error bars into the vertical direction. Finally, the fit is performed again using the new combined uncertainty. This produces both a value for adiabatic flame speed, $S_L$, and the value of its uncertainty, $\sigma_{S_L}$. The error propagation technique and the Method of Least Squares are described in detail in the text by Bevington and Robinson [20].
3.3.3 Equivalence Ratio Uncertainty

Next, consider the uncertainty in equivalence ratio caused by the uncertainty in the mass flow controllers. The ratio for a stoichiometric methane air flame is 9.52 mol of air for every 1 mol of CH₄. The equivalence ratio can then be written as:

$$
\Phi = \frac{\dot{V}_{CH_4}}{\dot{V}_{Air}}
\frac{1}{9.52}
= \frac{9.52\dot{V}_{CH_4}}{\dot{V}_{Air}}
$$

(3.17)

where \(\dot{V}_{CH_4}\) and \(\dot{V}_{Air}\) are the methane and air volume flow rates, respectively. Using propagation of error gives the following equation for the uncertainty in equivalence ratio:

$$
\sigma^2_{\Phi} = \left(\frac{9.52}{\dot{V}_{Air}} \sigma_{\dot{V}_{CH_4}}\right)^2 + \left(\frac{9.52\dot{V}_{CH_4}}{\dot{V}_{Air}^2} \sigma_{\dot{V}_{Air}}\right)^2
$$

(3.18)

Using this equation, it was determined that the mass flow controller uncertainty causes an uncertainty in equivalence ratio that ranges from 0.01 for the lean flames, up to 0.025 for the rich flames.

3.3.4 Air Oxygen Content Uncertainty

The last thing considered in this error analysis, is the composition of the gases used to create the premixed flames. The methane used was C. P. grade (chemically pure) and is better than 99% pure methane. This causes negligible effects on the mixture equivalence ratio. However, the oxygen content of the compressed breathing air cylinders used as the oxidizer has a larger uncertainty. The cylinders were purchased from General Air. When contacted, General Air reported that their compressed air can vary in oxygen content from 19.8-22% by volume. This would cause a
large uncertainty in the equivalence ratio of the flame reactions. To get a better idea of the composition of the air in the cylinders, an oxygen sensor was used to measure the oxygen content. The sensor has an absolute uncertainty of 0.1%. Measurements were taken from two of the cylinders used, and both came out to be 21% ± 0.1%. This uncertainty in oxygen content will not be included in the equivalence ratio error bars. This is because the equivalence ratio is calculated using the ratio of fuel to air. Changing the oxygen content of the air can be thought of as actually changing the oxidizer used in the reaction. Instead, the freely propagating flame code was used to investigate the influence that the altered oxygen content has on flame speed. Figure 3.5 shows the variation of flame speed with air oxygen content.

![Flame Speed vs. O2 Content for Φ = 0.7](image)

Figure 3.5. Flame Speed vs. O2 Content for Φ = 0.7

As shown in Figure 3.5, variation in O2 content of 0.5% results in a flame speed change of less than 0.5 cm/s. Our uncertainty in O2 content of 0.1% would result in less than 1 mm/s shift in flame speed, and is negligible when compared to the other experimental uncertainties. The authors of the experimental results that this study will be compared to, do not provide any information about the gases used in their flame speed measurements. Depending on the manufacturer and grade of the gases, the impurities could potentially have a significant effect on the quality of the flame
speed measurements. Future researchers should make sure that they know exactly what gases they are burning, and make it clear in any work that they publish.

Figure 3.5 shows flame speed increasing with the $O_2$ content of the mixture. This result is somewhat unexpected, because for a lean flame, one would expect higher oxygen content to further slow the flame speed. However, this can be explained by the fact that oxygen has a smaller specific heat than nitrogen. Figure 3.6 shows how the specific heat of the unburned mixture varies with oxygen content.

![Figure 3.6. $C_p$ vs. $O_2$ Content for $\Phi = 0.7$](image-url)
CHAPTER 4

RESULTS AND DISCUSSION

4.1 Flame Speed vs. Heat Loss

Figures 4.1 and 4.2 are plots of burner averaged flame speed vs. heat loss. The linear fit lines are displayed to illustrate which data points were used in extrapolating to laminar flame speed. The vertical error bars, $\sigma_{S_{ave}}$, decrease with slower flame speeds. This is because the uncertainty in burner averaged flame speed is dominated by the mass flow controller uncertainty, which is proportional to the flow rate. The horizontal error bars, $\sigma_{q_f}$, start out small and increase with heat loss. To understand why, take a look at Equation 3.15, the expression for heat loss in terms of the experimental parameters. Using partial derivatives, we can write expressions describing how each experimental uncertainty contributes to the overall uncertainty in the flame heat loss:

\[
\frac{\delta q_f}{\delta V_{H_2O}} = \frac{\rho_{H_2O} C_{p_{H_2O}} \Delta T_{H_2O}}{F_{CH_4}} \quad (4.1)
\]
\[
\frac{\delta q_f}{\delta \Delta T_{H_2O}} = \frac{\dot{V}_{H_2O} \rho_{H_2O} C_{p_{H_2O}}}{F_{CH_4}} \quad (4.2)
\]
\[
\frac{\delta q_f}{\delta F_{CH_4}} = -\frac{\dot{V}_{H_2O} \rho_{H_2O} C_{p_{H_2O}} \Delta T_{H_2O}}{F_{CH_4}^2} \quad (4.3)
\]

As you can see, Equations 4.1 and 4.3 both contain the term $\Delta T_{H_2O}$ in the numerator. Higher flame heat loss corresponds to a larger $\Delta T_{H_2O}$, and therefore, larger uncertainty in the heat loss measurement. Additionally, Equations 4.1, 4.2, and 4.3 contain the fuel flow rate in the denominator. As described in Section 3.1, the higher heat loss values are associated with smaller flow rates, and therefore, larger uncertainty.
Figure 4.1. Lean Flame Data

Figure 4.2. Rich Flame Data
4.2 Flame Model Comparisons

Figure 4.3 compares the experimental data to numerical data generated using GRIMech 3.0 [4]. As described in Section 3.3, the error bars on the extrapolated laminar flame speed values were generated using the Method of Least Squares. As one can see, the faster flames have much larger error bars than the slower flames. The main reason is that the slower flames required smaller mass flow controllers, which have a much smaller uncertainty. Also, the mass flow controller uncertainty is 1% of the flow reading, and the slower flames require lower flow rates.

![Figure 4.3. Comparison of Experimental Data to Flame Models](image)

GRIMech 3.0 was used as the input mechanism for two separate flame simulations to produce laminar flame speed data. The first, and most straightforward, is the freely propagating flame simulation in Cantera. In this simulation, the user supplies the gas composition, pressure, and initial temperature. The simulation returns the laminar
flame speed, along with profiles of temperature, species, and gas properties. The other simulation used is the burner stabilized flame simulation in Chemkin. This simulation is different because instead of initial gas temperature, the user supplies the burner surface temperature and the mass flux rate of the unburned gas. The flame speed value returned by the simulation is not the laminar flame speed. Instead, it returns the burner averaged flame speed with heat loss. Just like the heat extraction method, we can use this data to plot burner averaged flame speed vs. heat loss, and then extrapolate to zero heat loss to obtain the laminar flame speed. As described in Section 3.2, the burner heat transfer model is used to calculate the approximate burner surface temperature to input to each run of the simulation. The simulation was run at the same conditions as some of the flames of this study, essentially creating a simulated version of the experimental data.

As shown in Figure 4.3, the results from the two simulations are nearly identical, and are within the error bars of the experimental data for over half of the equivalence ratios. The model is not within the error bars for equivalence ratios of 0.7, 1.4, and 1.6. For \( \Phi = 0.7 \), the model over-predicts the experimental results by nearly 5 cm/s, or 3.5\( \sigma_{SL} \). For \( \Phi = 1.4 \), the model under-predicts the experimental results by nearly 7 cm/s, or 6.25\( \sigma_{SL} \). For \( \Phi = 1.6 \), the model also under-predicts the experiment, but is much closer, within 2\( \sigma_{SL} \). This will be discussed further in Section 4.3.2 because this trend can be seen when comparing the model to other literature data, including several of the target values used to optimize the mechanism for laminar flame speed prediction.

It is also interesting to compare the experimental flame heat loss with that predicted by the burner stabilized flame simulation. Figures 4.4 through 4.6 show these comparisons at three different equivalence ratios. For an attached, stoichiometric flame, the model closely predicts the flame heat loss. However, it greatly over-predicts the heat loss for lean flames, and under-predicts the heat loss for rich flames. This potentially highlights some shortcomings of the burner stabilized flame model. The model describes the ideal, undisturbed, laminar, burner stabilized flame. It does not take into account effects such as quenching on the burner surface, catalytic reactions inside the porous plug, and boundary layer effects near the edges of the flame. If the
Figure 4.4. Experiment vs. Burner Stabilized Flame, $\Phi = 0.6$

Figure 4.5. Experiment vs. Burner Stabilized Flame, $\Phi = 1.0$
methane is indeed reacting catalytically inside the burner plug, this would make the lean flames leaner and colder, and it would make the rich flames leaner and hotter. This could partially explain the deviation between the burner stabilized flame simulation and the real burner flames. However, if this were the only thing causing the deviations, the data would not line up for a stoichiometric flame, rather, they would most likely match slightly on the rich side. Clearly, there are many mechanisms at work, and there is not enough data to draw or test any firm conclusion.

Another possible explanation for the deviations in heat loss values could be problems with GRIMech 3.0 itself. As will be discussed in Section 4.3.2, the mechanism calculates lean flame speed values that are significantly higher than the experimental data, as well as almost all literature data. This would explain why burner stabilized flame over-predicted the heat loss for the lean flames. Faster flame speed is associated with a hotter flame, and it would bring the flame closer to the burner surface, increasing the heat transfer rate. Similarly, the mechanism significantly under-predicts experimental and literature flame speed data for rich flames. This would explain why burner stabilized flame under-predicted the heat loss for the lean flames, because
slower flames are cooler, and would stand further away from the burner, causing lower heat transfer rates. This will be discussed further in Section 4.3.2.

Another difference between the burner stabilized flame simulation and real flames, is that the simulation under-predicts the heat loss for the higher flow rate flames that stand off from the burner surface. In practice, as the flow rate increases and the flame begins to blow off, the flame becomes wrinkled, increasing its surface area. This allows the flame to stay close to the burner. However, the simulation does not take this effect into account, causing it to calculate a higher standoff distance, and a much smaller rate of heat transfer to the burner. This also causes the simulation to fail to find a converged solution when the gas velocity nears the adiabatic flame speed. However, the increased flame area caused by these stretching effects allows a real flame to be established with the gas velocity more than 25% higher than the adiabatic flame speed.

4.3 Literature Data Comparisons

It is difficult to compare the results of this study to existing literature data. This is because the experiment was carried out in Golden, CO, elevation 5,676 ft. Ambient pressure in Golden is roughly 81% of atmospheric pressure at sea level. Most published flame speed data is from experiments performed at or near sea level. It is therefore necessary to come up with a way to scale the experimental data from pressure in Golden, to atmospheric pressure at sea level. At a minimum, this will allow a qualitative comparison between the experimental data and literature data.

4.3.1 Flame Speed vs. Pressure

Egolfopoulos et al. [21] used the twin counter flow method and a pressure chamber to measure methane-air adiabatic flame speed vs. equivalence ratio, at a variety of pressures. Figure 4.7 shows their flame speed data. C. K. Law, one of the researchers,
went on to publish a paper in 1993, which states that this data is an overestimate by as much as 10%. This is because the jets were too close together, resulting in high strain rates in the flames used for extrapolation to adiabatic flame speed. It was found that placing the jets farther apart, and using flames with lower strain rates, produces more accurate values of flame speed [22]. An additional problem is that the authors did not include error bars in their data. They performed the experiment several times and determined that they have a repeatability of 1-2 cm/s. However, this still does not describe how accurate the measurements actually are.

![Flame speed data from Egolfopoulos et al. 1994](image)

Figure 4.7. Flame speed data from Egolfopoulos et al. 1994

Even though this data is off by as much as 10%, it can still be used to examine how flame speed varies with pressure. There are curves for .25, .5, 1, 2, and 3 atm. We can rearrange this data to plot flame speed vs. pressure at each equivalence ratio. Fitting curves to each of these plots provides expressions for flame speed in terms of pressure, at each equivalence ratio. These expressions can then be used to scale the experimental data from pressure in Golden, to atmospheric pressure at sea level. As described in the textbook by Glassman [1], it is known that flame speed scales as:

$$ S_L \sim (P^{(n-2)})^{1/2} $$

(4.4)
where $P$ is the pressure, and $n$ is the order of the reaction. It is therefore logical to use power law fits to calculate the pressure scale factors. That way, each fit equation will be of the same form as the theoretical expression for the pressure scaling of laminar flame speed. The power law fits are of the form:

$$S_L = AP^n$$  \hspace{1cm} (4.5)$$

where $A$ is the pre-exponential coefficient, and $q$ is the exponent in the power law fit. With these fit equations, we can calculate scale factors to translate the experimental data to atmospheric pressure. The curve fitting functions in Matlab were used to perform the power law fits. A 95% confidence interval was calculated for the value of $q$, which we can use to put error bars on the scale factors. We can then use the following expressions to scale the data to atmospheric pressure at sea level:

$$S_{L_{sea\ level}} = \frac{S_{L_{Golden}}}{ScaleFactor}$$

$$ScaleFactor = \frac{S_{L_{Golden}}}{S_{L_{sea\ level}}} = \frac{AP^n_{Golden}}{AP^n_{sea\ level}}$$

$$ScaleFactor = \frac{P^n_{Golden}}{P^n_{sea\ level}}$$  \hspace{1cm} (4.6)$$

where $P_{Golden}$, $S_{L_{Golden}}$, $P_{sea\ level}$, and $S_{L_{sea\ level}}$ are the pressure and laminar flame speed in Golden and at sea level, respectively.

Now that we have an expression for the scale factors, we can use the confidence intervals on the $q$ values, along with propagation of error, to place error bars on the scale factors. We get the following expression for scale factor uncertainty:

$$\sigma_{ScaleFactor} = P^n \ln P \sigma_q$$  \hspace{1cm} (4.7)$$

where $\sigma_q$ is equal to half of the confidence interval placed on $q$. The scale factor error
bars can then be combined with the error bars on the experimental data, giving us the following expression for total uncertainty of the scaled experimental data:

\[ \sigma_{S_{\text{sea level}}} = \sqrt{\left(\text{ScaleFactor} \cdot \sigma_{S_{\text{Golden}}} \right)^2 + \left(\frac{-S_{\text{Golden}}}{\text{ScaleFactor}^2} \cdot \sigma_{\text{ScaleFactor}}\right)^2} \quad (4.8) \]

Figure 4.9, shows the scaled data and error bars, along with literature and model data. The figure will be discussed in detail in Section 4.3.2.

We can also use this information to get an idea of how the reaction order varies with equivalence ratio. From Equations 4.4 and 4.5, it is clear that the reaction order can be written as:

\[ n = 2q + 2 \quad (4.9) \]

and the reaction order uncertainty can be written as:

\[ \sigma_n = 2\sigma_q \quad (4.10) \]

Figure 4.8 is a plot of reaction order vs. equivalence ratio. The reaction order peaks at a value of 1.27, at an equivalence ratio of 1.1. Near the lean flammability limit, the reaction order drops off to a value of approximately 0.55. At \( \Phi = 0.6 \), the reaction order goes negative. This point is not shown on the chart because it is not a physically valid result. While the reaction order may approach zero, it would never go negative. The cause for this problem is that there are not enough data points at \( \Phi = 1.5 \) and 1.6 to perform the power law fits of flame speed vs. pressure. Instead, plots were made of the other scale factors and scale factor uncertainties, and the values for \( \Phi = 1.5 \) and 1.6 were obtained by extrapolating. Lower reaction order means that the propagation of these weaker flames is affected by ambient pressure much more than the flames closer to \( \Phi = 1. \)
4.3.2 Flame Speed vs Equivalence Ratio

Now that the experimental adiabatic flame speed data has been scaled to atmospheric pressure, it can be compared to literature data. Figure 4.9 displays the experimental data, along with data from various research groups, each using different methods of measuring flame speed. Additionally, the figure includes flame speed calculated using the adiabatic freely propagating flame simulation with GRIMech 3.0 as the input reaction mechanism, denoted on the plots as GRIMech 3.0 FPF.

Law, Vagelopoulos, and Egolfopoulos

C. K. Law and C. K. Wu developed the twin counterflow technique in 1984. Since then, Law has collaborated with C. M. Vagelopoulos and F. N. Egolfopoulos on numerous flame speed studies using the twin counterflow technique. Figure 4.9
Figure 4.9. Literature Flame Speed Comparison

includes the experimental data from Vagelopoulos et al. 1994 [23]. This data was published shortly after Law published the 1993 paper [22] that described how previous flame speed measurements using the twin counterflow flame technique were too high. The technique was improved by using larger jet separation distances, as well as lower flame strain rates. Although no discussion of error analysis is provided, they claim a repeatability of 1-2 cm/s. In 1998, Vagelopoulos and Egolfopoulos published their paper on the stagnation plane method [9]. This method is discussed in Chapter 2. The authors believe this method to be even better than the improved counter flow method, because it directly measures the laminar flame speed, without a strain rate extrapolation. Though not shown in Figure 4.9, these flame speed values are between 1 and 2 cm/s slower than the values from Vagelopoulos et al. 1994. This makes the stagnation plane results very close to the experimental values from the current study for lean flames. However, on the rich side, the stagnation plane results are even further away from the results of the current study, as well as other literature data.

The experimental data from Vagelopoulos et al. 1994 agree with the results of the current study to within error bars for equivalence ratios that are near stoichiometric.
However, for very rich flames, the 1994 results claim flame speed values that are up to 5 cm/s slower than the data from the current study, as well as most other literature data. Not surprisingly, the flame speed values from the GRIMech 3.0 freely propagating flame simulation follow this trend. This is because the $\Phi = 1.43$ flame speed value from Vagelopoulos et al. 1994 was used as a target value to validate GRIMech 3.0. It is difficult to decide which of these flame speed values are the most accurate for the richest equivalence ratios. The twin counterflow method, when used with sufficiently low strain rates, can be very accurate. Most of the other recent literature data has come from flat flame methods. The twin counterflow method has much less chance of catalytic reactions and quenching affecting the flame, because the flames stand much farther away from the nozzles than they do for a flat flame burner. Additionally, the strained flame speed measurements are taken using particle tracking techniques. This allows the direct measurement of strained flame speed near the center of the flame, where the flame is not disturbed by boundary layer effects. Flat flame methods, however, measure the burner averaged flame speed across the flame surface by dividing the volume flow rate by the burner surface area, capturing the boundary layer effects in the flame speed measurement. The largest downfall of the studies published by the Law, Egolfopoulos, and Vagelopoulos, is that they do not provide any kind of uncertainty values for the flame speed measurements. Even though they claim a repeatability of 1-2 cm/s, it is hard to put much faith in the quality of the measurements without some idea of the absolute uncertainty. It is easier to trust the data from the flat flame methods, because both experiments have been put through a detailed uncertainty analysis.

**Bosschaart and DeGoey**

K. J. Bosschaart and L. P. H. de Goey used the heat flux method to measure flame speed [11]. The heat flux method is very similar to the heat extraction method. The way in which the flames attach to the burner, as well as any possible quenching, catalytic reactions, and edge boundary layer effects, are nearly identical. Perhaps this is why their 2003 data is so close to the results of this study. Their data agrees with the results of the current study at every equivalence ratio. Bosschaart and de Goey
performed an error analysis, providing both flame speed and equivalence ratio error bars. These error bars are only depicted for flames of $\Phi = 0.75$ and leaner, and for $\Phi = 1.3$ and richer. This is because the data points and error bars were taken from the chart in their 2003 paper, and the near-stoichiometric error bars are smaller than the symbol size on the chart.

**Andrews and Bradley**

Andrews and Bradley used the double kernel technique described in Section 2.2.1. As described, the two flames must be ignited simultaneously, and Andrews and Bradley were only able ignite them within a few milliseconds of each other. Also, the flame fronts would often propagate obliquely to the camera, causing it to appear as though the flames had already met, when in fact, they still had significant distance to propagate. These complications result in flames speed measurements that are too high, and most likely explain why this data is significantly higher than data published by other research groups.

**GRIMech 3.0**

As described above, GRIMech 3.0 seems to over-predict the lean flame speeds, and under-predict the rich flame speeds. This is not surprising for the rich flames, because the target value used to optimize the mechanism for rich flame speeds is roughly 5 cm/s lower than the other literature data. For lean flames, however, the target values agree with the other literature, but the mechanism misses the target values entirely, over-predicting them by 2-3 cm/s.

As described in Section 4.2, GRIMech 3.0 used with the burner stabilized flame simulation has difficulties predicting the heat transfer to the burner for the lean and rich flames. It is likely that the burner stabilized flame heat transfer errors are di-
rectly related to the GRIMech 3.0 flame speed errors. On the lean side at phi 0.67, the GRIMech 3.0 flame speed is 25% over-predicted from the mean of the literature and current experimental data. This is about a two sigma over-prediction from the experimental mean. At this equivalence ratio, the heat transfer is over-predicted by burner stabilized flame and GRIMech 3.0 by about a factor of two. These deviations correspond because the faster flame speed at the same reactant mass flux causes the calculated stand off distance to be smaller, thus increasing the calculated heat transfer. On the rich side, GRIMech 3.0 under-predicts flame speed by nearly 28% relative to the mean of the literature and experimental data. This is also roughly two sigma uncertainty. At this equivalence ratio, burner stabilized flame and GRIMech 3.0, under-predict the heat transfer by as much as 50%. These deviations correspond because a slower flame speed at the same reactant mass flux would cause the calculated standoff distance to be larger, thus decreasing the calculated heat transfer. Near stoichiometric conditions, both the GRIMech 3.0 flame speed predictions, and the burner stabilized flame heat transfer predictions, match the experiment to within the error bars. This strongly suggests that the poor burner stabilized flame predictions are directly related to the poor flame speed predictions of GRIMech 3.0, and are not a result of the simplicity of the burner stabilized flame model.

**Smoothed Spline Fit**

In an attempt to come up with a curve representing the best flame speed values, a smoothed spline fit was done that combines the data from Vagelopoulos *et al.* 1994, Bosschaart *et al.* 2003, and the current study. This curve can be thought of as the “mean” of the best available experimental results. The fit was done in Matlab, using CSAPS, the cubic smoothing spline function in the non parametric fitting toolbox. This fitting tool uses a smoothing parameter, $p$, which varies between 0 and 1. A $p$ value of 0 produces a least squares linear fit, and a value of 1 produces a cubic spline. The parameter can either be specified, or Matlab will determine the best value automatically. For this fit, the parameter was determined by Matlab, and came out to be $p = 0.999802$. As shown in Figure 4.9, the fit closely follows both the experimental data from this study, and the Bosschaart *et al.* data.
Figure 4.10. Residual Plot (Percent Deviation)

Figure 4.11. Residual Plot (Absolute Deviation)
Now that we have a curve representing the best flame speed values, we can create residual plots showing the amount by which the rest of the data deviates from this optimum flame speed curve. This will help to further emphasize and quantify the deviations shown in Figure 4.9. Displayed above, Figure 4.10 is a plot of the deviation from the smoothed spline fit in percent, and Figure 4.11 is the same plot with absolute deviations in m/s. As shown in Figure 4.10, freely propagating flame with GRIMech 3.0 starts off at $\Phi = 0.6$ by over-predicting by 26%, and then improves as $\Phi$ approaches stoichiometric. However, as shown in Figure 4.11, the worst prediction on the lean side in terms of absolute value occurs at $\Phi = 0.8$, where it over-predicts by more than 3 cm/s. On the rich side the worst prediction, both in terms of percentage and in absolute value, occurs at $\Phi = 1.4$, with an under-prediction of 27.5%, or more than 5 cm/s. At $\Phi = 1.43$, the GRIMech 3.0 target value is low by more than 24%, or roughly 4 cm/s. Although the Vagelopoulos et al. data point at $\Phi = 1.1$ is outside the error bars of this study, it deviates from the mean only slightly more than this study, less than 5%. If error bars had been placed on the Vagelopoulos data, they would likely overlap with the error bars from this study, bringing the two data points into agreement.
CHAPTER 5

CONCLUSIONS

The main focus of this thesis was to evaluate the accuracy of the heat extraction method for measuring laminar flame speeds. This was done by developing a simple heat transfer model to help determine the validity of assumptions made in using this method, and by carefully documenting all sources of experimental uncertainty to include in a detailed error analysis. Also, the experimental results were compared to various sources of literature data, as well as model results generated using GRIMech 3.0. The experiment was found to agree well with much of the literature data.

This study has highlighted some significant shortcomings of GRIMech 3.0, with regards to flame speed prediction. The mechanism accurately predicts flame speed over the range of equivalence ratio from $\Phi = 0.9$ to $\Phi = 1.2$. However, its predictions of rich and lean flame speeds, deviate from accepted values by as much as 25%. This study also points out some shortcomings of the burner stabilized flame simulation. The simulated heat transfer values severely deviate from the experiment for rich and lean flames, being off by as much as a factor of two. As described in Section 4.3.2, this is mainly a result of the problems with the rich and lean flame speed predictions of GRIMech 3.0. However, it should be pointed out that the burner stabilized flame model fails to account for phenomena that occur in real burner stabilized flames, such as quenching effects, catalytic reactions inside the burner plug, and boundary layer effects at the flame edges. No attempt is made to quantify the effect that these phenomena have on the measured laminar flame speed values, but all of these phenomena disturb the flame, causing it to deviate from the ideal, laminar, burner stabilized flame. Possible future work could include modifying the burner stabilized flame model to include the burner surface. It should include the heat conduction through the metal, as well as surface chemistry and quenching effects. This would go a long way towards making the model closer to describing a real flame.
Another problem that is true of almost all flame simulations, is that the simulated data contains no error bars. Uncertainty could reasonably be placed on all of the reaction rate constants and other data present in a reaction mechanism. Then, the simulation could be solved numerous times, each time varying one of the input parameters, and saving the results. This would be repeated for every input parameter, until a total uncertainty can be placed on each output value of the flame simulation. On an average desktop computer, this would take days, or even weeks to complete one run of the simulation. However, as computers become faster, a simulation of this kind will become more practical, and could prove to be very useful.

Additionally, this study has highlighted some possible shortcomings of the flat flame methods. Edge effects from the boundary layers, as well as surface effects from the porous plug, work to further deviate the flame from the ideal adiabatic laminar flame. This has an effect on the outcome of the flame speed measurements. Bosschaart et al. claim that the heat flux method is superior, because it does not require an extrapolation to measure the adiabatic flame speed. However, their results are nearly identical to the results of this study, which uses a heat loss extrapolation. This suggests that using a heat loss extrapolation is, in fact, a valid approximation, and that the boundary layer, quenching, and catalytic effects, have a much larger effect on the flame speed measurements.

The twin counterflow method avoids many of these effects. The large stand-off distance of the flames from the nozzle helps to eliminate catalytic reactions and quenching effects. Additionally, the strained flame speed is directly measured with a particle tracking technique, rather than finding the average flame speed over the entire flame area. This avoids the boundary layer effects at the edge of the flame, because the velocity can be measured near the center of the flame disk, where the reaction is much closer to an ideal, adiabatic, laminar flame. However, the 1998 stagnation flame method study by Vagelopoulos and Egolfopoulos suggests that even the improved counter flow method with lower strain rate slightly over-predicts laminar flame speed. Their data from the stagnation plane method is 1-2 cm/s slower than the data from the counterflow method, at every equivalence ratio. This brings the value into close agreement with the results of this study for lean flames, but causes them to deviate
even further for rich flames. Also, the uncertainties of these methods have not been investigated. It would be very interesting to see a detailed error analysis performed on these methods in order to get some idea of their absolute uncertainties. The stagnation plane and counter flow flame methods involve a very complicated apparatus. Given the current information, there is no evidence that either of these methods provide higher accuracy than the flat flame methods. Unless a detailed uncertainty analysis is performed and proves otherwise, the flat flame methods provide the best balance between accuracy and simplicity for measuring laminar flame speed.

Finally, this study has pointed out the lack of reliable experimental data relating pressure to laminar flame speed. Egolfopoulos' data was used to scale the experimental values to atmospheric pressure at sea level. Theoretically, laminar flame speed scales as \( S_L \sim (P(n-2))^{1/2} \) and should closely fit the form of a power law fit curve. However, Egolfopoulos' data is very scattered, and most equivalence ratios do not fit the power law form. This causes large error bars on the scale factors used to convert the experimental data from pressure in Golden, to sea level atmospheric pressure. Additionally, the Egolfopoulos data was used to optimize the pressure variation of GRIMech 3.0, suggesting possible problems with this aspect of the mechanism. Shortly after Egolfopoulos published this data, the counter flow flame method was improved. It would be greatly beneficial to repeat his experiment using the improved technique, or possibly the stagnation plane technique. It would also be useful to repeat the current study, with the burner placed inside a pressure chamber. The heat extraction method could then be performed at atmospheric pressure, allowing for direct comparison to literature data, without scaling for pressure effects.
REFERENCES CITED


