FY 2017 Progress Report:
Adiabatic Flame Temperature and Equivalence Ratio Relationship

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1 Major Accomplishments

The team was able to find the adiabatic flame temperature that corresponds to different equivalence ratio. By comparing the flame temperature, an optimal equivalence ratio could be chosen. Therefore, this optimal equivalence ratio could be used in future experiments where high flame temperature is needed.

2 Project Objectives

The purpose of this study was to investigate the dependence of adiabatic flame temperature on equivalence ratio for a variety of fuels and compare experimental and theoretical methods for calculating adiabatic flame temperatures. Since adiabatic flame temperature is a good measure of a fuel's chemical energy content, it is desirable to find the equivalence ratio which maximizes the adiabatic flame temperature. The equivalence ratio defines the proportion of fuel to oxidant in the combustion mixture and can be varied by adjusting air or fuel flow rates. The current study experiments with methane/air mixtures to study these relationships.

This study begins with a brief overview of the experimental set-up and experimental and theoretical methods. The results are presented in the discussion section and important trends, possible error, and conclusions are discussed.

3 Experimental Set-up

The experimental set-up includes methane and compressed air tanks, needle valves, flow rate meters, a conical flame produced by a Bunsen burner, and a thermocouple attached to a data acquisition device to measure the temperature of the flame front as shown in figure 1 on page 4. A thermometer and barometer measure the local room temperature and pressure. The methane and air flow rates through tubing can be adjusted using needle valves and flow rate meters. Varying the flow rates of the reagents changes the equivalence ratio. The position of the thermocouple junction of the thermocouple can be adjusted to locate the hottest portion of the conical flame by maximizing the voltage from the data acquisition display. The hottest portion of the flame corresponds to the flame zone. This conical flame and premixing approximates the conditions of real-world applications. The data can then be recorded on a computer for analysis.

Protective glasses are worn to avoid radiation to the eyes, and safety measures were taken to prevent methane pressure built up in the gas tanks.

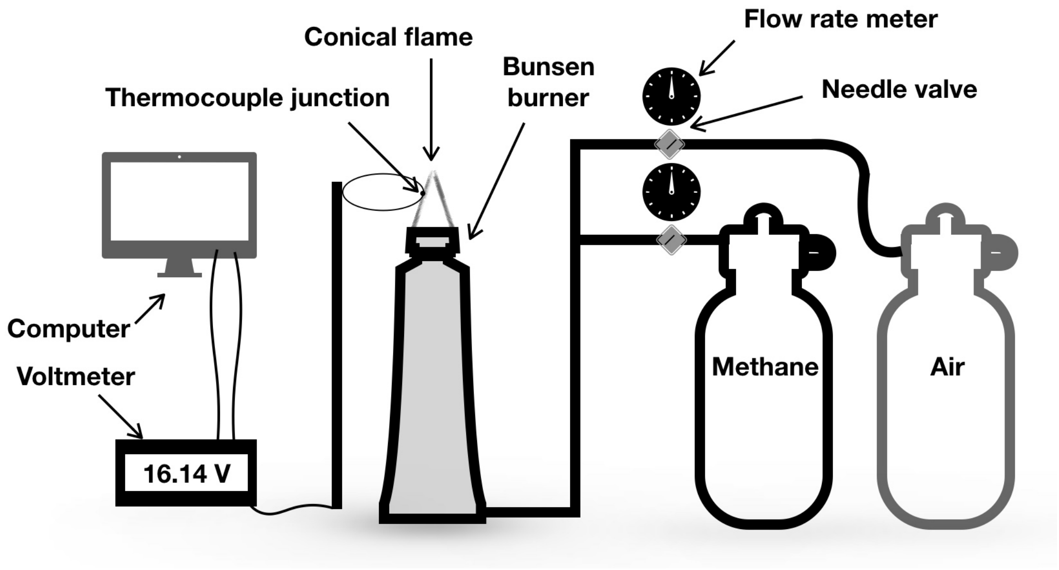

Figure 1: Experimental Set-up. Shut-off valves not shown.

4 Methodology

4.1 Finding Adiabatic Flame Temperature from Experimental Data

Experimental data obtained are mainly $E(Tm)$, the emf of the thermocouple read from the voltmeter, and also the equivalence ratio, ϕ, which can be varied by altering the flow rates of methane and air. The temperature of the thermocouple junction, T_j, can be estimated from $E(Tm)$ using tabulated thermocouple data. The temperature and pressure of the surrounding room are T_s and P_s, respectively. The adiabatic flame temperature is the temperature of the air-gas mixture at which combustion is allowed to proceed adiabatically at constant pressure. The temperature of the products, T_g, can be approximated by accounting for radiation losses at the thermocouple junction. Although T_a is the temperature of interest, T_g is easier to calculate and can be assumed to be equal to T_a.

4.2 Theoretical Results from STANJAN

Theoretical adiabatic flame temperature values, $T_{Stanjan}$, were obtained from STANJAN simulation software. The software begins with an initial guess of the adiabatic flame temperature temperature T_{a1}. STANJAN then determines what the equilibrium composition of products minimize the Gibbs free energy at T_{a1} and the given pressure. The total enthalpy for that composition is then compared to the enthalpy of the reactants at the known initial reaction temperature. STANJAN then iterates with new values of T_{a2}, T_{a3}, etc. until the enthalpy of the reactants equals the enthalpy of the products.

The inputs needed to use STANJAN include the initial reaction pressure, the involved elements, the reactant species and mole fractions, the product species, and the choice of which parameters remain constant (in the case of this experiment, pressure and enthalpy). The mole fractions of the reactants were found using the corrected flow rates from the data collection spreadsheet of each reactant species. Later calculations assume that $T_a = T_{Stanjan}$.

4.3 Radiative Heat Transfer Correction for Junction Temperature

The junction temperature is not equivalent to the product gas temperature. At steady state, there is an energy balance between radiative and conductive losses and convection from the flame. However, conductive losses can be neglected since the cross-section of the thermocouple wire is small and convective and radiative heat transfer modes are much more significant. After solving for T_g, the balance of convection and radiation is thus:

$$T_g = T_j + \frac{\epsilon\sigma}{h}(T_g^4 - T_j^4) \tag{1}$$

where
ϵ: the emissivity of the thermocouple wire. This value is estimated from Touloukian's [3]
σ: 5.67x10e-8 $Wm^{-2}K^{-4}$ the Stefan-Boltzmann constant
h: the heat transfer coefficient of the air.

The heat transfer coefficient is calculated from a Nusselt number correlation, and gas properties are evaluated at the film temperature, $T_f = \frac{T_j+T_g}{2}$ where T_g is estimated as $T_{Stanjan}$:

$$Nu = \frac{hd}{k} = (0.24 + 0.56Re_d^{0.45})(\frac{T_f}{T_g})^{0.7} \tag{2}$$

k: thermal conductivity of the gas products
d: diameter of thermocouple wire
$Re_d = \rho$Vd$/\mu$: the Reynolds number for the flow.
V: average reactant velocity. This value is used to approximate the product velocity.
ρ: density of gas mixture
μ: viscosity of gas

5 Results and Discussion

5.1 Radiation Correction

The junction temperatures were smaller than the calculated gas temperatures. This is because the thermocouple junction and gas products are not in thermal equilibrium as described above in the methods section. Chemical reactions on the junction surface provided convective heat addition, and heat was lost through thermocouple radiation to the surroundings. Conduction losses can be neglected since the cross-sectional area of the thermocouple wire is small. The effects of the radiation correction are most significant as the gas temperature reaches a maximum.

However, the radiation correction is not ideal. The system is assumed to be in steady state, but with the flame movement and thermocouple positioning, this may not be a valid assumption. The thermocouple wire is approximated as an infinite cylinder. The adiabatic temperature in the Nusselt correlation is approximated with the STANJAN result. Further, other Nusselt valid correlations [4] differ by up to 12%.

5.2 Method Comparison: Theory and Experiment

5.3 Method Limitations and Error

In the experiment, an assumption was made that the air and fuel are mixed perfectly for combustion. In reality, air and fuel are mixed simply by merging the two tubes. It is uncertain that fuel and air are combusted as much as possible. A quick way to validate this assumption is to add a air stirrer at merging point while controlling all other parameters, and then compare the resulting flame temperature. If there is no difference or it is negligible, then this assumption is valid.

Another uncertainty in the method is that the data may not have been taken at the maximum voltage. This was very dependent on human error, and was not necessarily consistent across the experiment. In our data there is a similarity between the measured values in the second and third trials, but not from the first trial (Figure 2). When partnering with another group, one half took the data for the first trial and the other took the data for the second and third. This human variation may explain the disparity in values between the first trial and the second and third trials.

6 Future Work

An automated positioning system could be developed to find the maximum temperature such that the thermocouple is always at the vertex of the conic flame, reducing the uncertainty from human error. In addition, other fuels and combinations of fuels can be tested, and maximizing equivalence ratios determined.

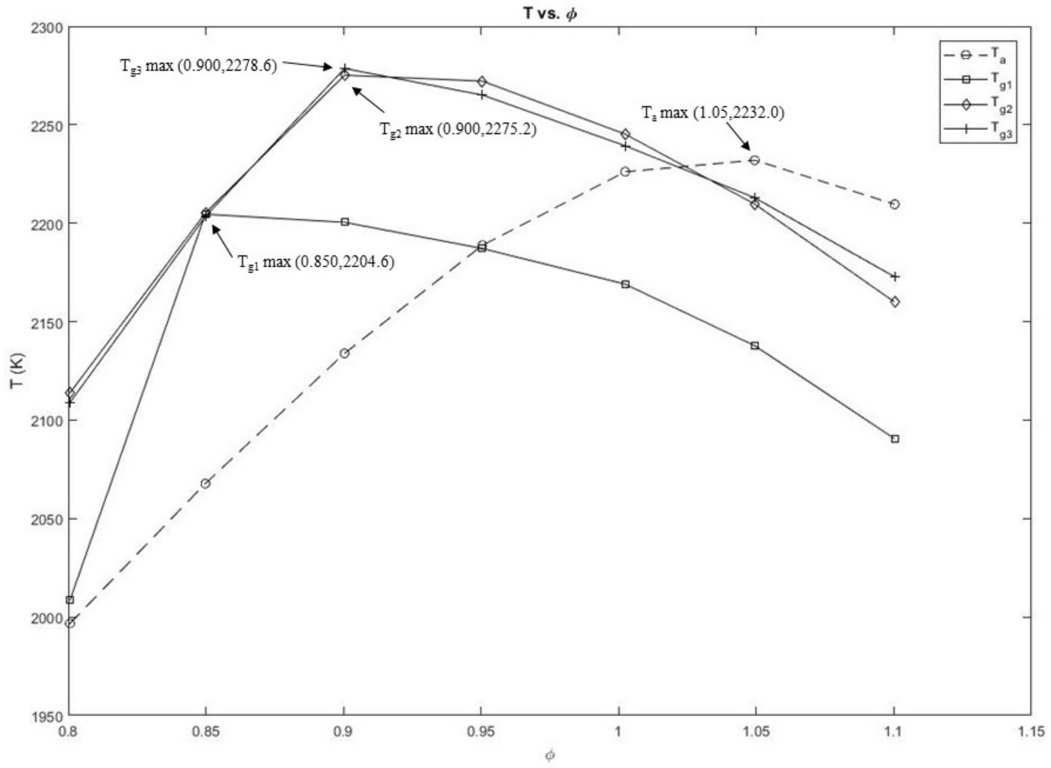

Figure 2: Plot of temperature vs. equivalence ratio.

Analysis via STANJAN and the experimental data yielded different maximum temperatures of the products as well as different equivalence ratios where the maximum temperatures occurred. The temperature from the experimental data peaked on the lean side of the equivalence ratio curve in each of the three trials, with the first trial producing a curve very different from the curves from the second and third trials. This could be attributed to the personnel change during the experiment; the roles performed by each individual remained the same during the second and third trials.
Unlike the experimental curves, the STANJAN curve peaks at a rich equivalence ratio and at a lower overall temperature. The maximum temperature calculated by STANJAN differs by only 0.93% from the average of the experimental maximum temperatures, however. It is unclear exactly what caused the shift of the experimental curve toward a maximum temperature with a lean mixture. It should be noted that certain gas mixtures and reacting with certain oxidants (F_2 for example) can cause such a shift. This is not likely to be the case in this experiment, but it is possible that some contaminant in the air or in the fuel could have shifted the results.

7 References

1. MAE 4272 Fall 2017 Lab Manual, HT1.
2. Collis, Williams and Haoyun, *J. Fluid Mechanics* 6, 357, 2056.
3. Touloukian, Y. S. (edt.), *Thermophysical Properties of High Temperature Solid Materials*, Vol. 1, Macmillan,
4. Frank P. Incropera, David P. DeWitt, *Introduction to Heat Transfer*, 2nd Edition, John Wiley and Sons: 1990. New York, 1967