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Adiabatic Flame Temperature for Combustion of Methane II

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Abstract

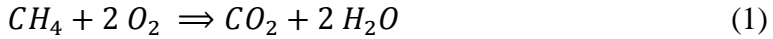
We calculate the adiabatic flame temperature of a mixture of methane and oxygen in the presence of a diluent gas then determine the mole fractions of methane without respect to nitrogen and solve for the moles of oxygen present. Knowing the moles of methane and oxygen, allows us to calculate the moles of nitrogen present at four constant mole fractions of nitrogen, and the adiabatic flame temperature is determined from the energy released by the reaction. Lastly, we produce several graphs to compare the adiabatic flame temperatures at different mole fractions of nitrogen.

Keywords

Methane, Combustion, Adiabatic Flame Temperature

PROBLEM STATEMENT

Methane (CH_4) combusts according to:



The goal of this project is to calculate the adiabatic flame temperature T_A for this reaction as a function of molar composition. The feed stream consists of methane, nitrogen and oxygen at 25°C. The calculation of the adiabatic flame temperature assumes that all of the heat liberated by the combustion reaction goes into heating the resulting mixture. The energy liberated by the reaction is given by:

$$(n_{CH_4}^0 - n_{CH_4}) \Delta H_c \quad (2)$$

where $n_{CH_4}^0$ is the moles of methane fed, n_{CH_4} is the moles of methane that did not combust, and ΔH_c is the heat combustion of methane at 25°C. Note that:

$$\Delta H_c = 802.3 \text{ kJ per mole of methane reactant.} \quad (3)$$

The energy that goes into heating the product gas is given by the following:

$$\begin{aligned} n_{CH_4} \int_{25}^{T_A} C p_{CH_4} dT + n_{O_2} \int_{25}^{T_A} C p_{O_2} dT + n_{CO_2} \int_{25}^{T_A} C p_{CO_2} dT \\ + n_{H_2O} \int_{25}^{T_A} C p_{H_2O} dT + n_{N_2} \int_{25}^{T_A} C p_{N_2} dT \end{aligned} \quad (4)$$

where the n_i represent the moles of species i that exist after the reaction occurs and the $C p_i$ are the heat capacities of each gas participating in the reaction. For the purposes of this project, the heat capacities can be assumed to be linearly dependent on temperature:

$$C p_i = A_i + B_i T \quad (5)$$

With the values of A_i and B_i given in the following table:

<i>Gas</i>	<i>A</i>	<i>B</i>
CH_4	0.034	2.50×10^{-6}
O_2	0.03	3.00×10^{-6}
CO_2	0.04	9.70×10^{-6}
H_2O	0.033	5.50×10^{-6}
N_2	0.037	2.20×10^{-6}

Construct a graph of T_A versus mole fraction on a triangular diagram where the vertices represent pure CH_4 , pure N_2 and pure O_2 . Use curves on the graph to represent lines of constant T_A .

MOTIVATION

Accurately calculating the adiabatic flame temperature of a combustion reaction is relevant to fields that deal with explosions or combustion reactions, for example, material production industries, demolitions, and chemical engineering fields. The adiabatic flame temperature of a reaction is the temperature of the products (or mixture of reactants, leftover products, and diluents) of a combustion reaction when all of the energy liberated by the combustion goes into heating the products.

Additionally, it is unlikely that a mixture of reactants will be 100% free of diluents when combusting. A diluent does not participate in the combustion and thus does not give off any energy in the reaction, it just serves to absorb heat and lower the overall adiabatic flame temperature. While it is ideal to have a mixture of pure combustive reactants to achieve the highest resulting adiabatic flame temperature, it is useful to be able to calculate how much diluent can be present while still reaching the desired adiabatic flame temperature.

The goal of this project is to explore what happens to the adiabatic flame temperature of a combustion reaction between methane and oxygen in the presence of a diluent gas, nitrogen. Several amounts of nitrogen were evaluated, including a mixture of nitrogen, methane, and oxygen that was 80% nitrogen. The composition of air is approximately 80% nitrogen, 19% oxygen, and 0.002% methane (along with other diluent gasses). While this is not the goal of the project, the results could also be used to extrapolate the theoretical adiabatic flame temperature for a mixture of nitrogen, methane, and oxygen similar to those present in air.

This project expands upon the recommendations of previous work found in the Undergraduate Journal of Mathematical Modeling (Pupo) which explored the adiabatic flame temperature of a mixture of pure methane and oxygen. By contrast, this project addresses the adiabatic flame temperature of methane reacting with air instead of pure oxygen.

MATHEMATICAL DESCRIPTION AND SOLUTION APPROACH

The first step in this project is to determine the mole fractions of methane and oxygen before being combusted on a nitrogen-free basis. This is done using the equation:

$$Y' = \frac{n_{CH_4}^0}{(n_{CH_4}^0 + n_{O_2}^0)} \quad (6)$$

In (6) we have $n_{CH_4}^0$ representing the moles of methane present before combustion, $n_{O_2}^0$ representing the moles of oxygen present before combustion and $0.05 \leq Y' \leq 0.95$ increasing in increments of 0.05. The initial moles of methane for each mole fraction is held constant with $n_{CH_4}^0 = 1$, so this equation is dependent on $n_{O_2}^0$. An example of this calculation is as follows:

$$0.05 = \frac{1 \text{ mol } CH_4}{1 \text{ mol } CH_4 + n_{O_2}^0}$$

$$0.05(1 + n_{O_2}^0) = 1 \tag{7}$$

$$n_{O_2}^0 = 19$$

The values of the moles of methane and oxygen for each Y' -value is provided in the chart in Section 1 of Appendix A.

After calculating the amount of methane and oxygen present on a nitrogen free basis, the amount of nitrogen present for each Y_{N_2} should be calculated. This is done by setting $0.2 \leq Y_{N_2} \leq 0.8$ in increments of 0.2, and using the equation:

$$Y_{N_2} = \frac{n_{N_2}}{n_{CH_4}^0 + n_{O_2}^0 + n_{N_2}} \tag{8}$$

where Y_{N_2} is the mole fraction of N_2 and n_{N_2} the number of moles of nitrogen present for that particular mole fraction. Because nitrogen will not participate in the combustion, n_{N_2} is constant, thus (7) is solved for n_{N_2} . For example with $Y_{N_2} = 0.2$ (7) becomes:

$$Y_{N_2} = 0.2 = \frac{n_{N_2}}{1 \text{ mol } CH_4 + 19 \text{ mol } O_2 + n_{N_2}} \tag{9}$$

Hence,

$$5 = n_{N_2} \tag{10}$$

The values of n_{N_2} for every mole fraction of methane and oxygen with $Y_{N_2} = 0.2, 0.4, 0.6, 0.8$ are given in Section 2 of the Appendix.

Once n_{N_2} is known, the values Y_{CH_4} and Y_{O_2} (the mole fractions of methane and oxygen respectively, with respect to the presence of nitrogen) can be calculated for each mole fraction at every Y_{N_2} . These values will be used later to create the triangular (ternary) diagram by plotting values of Y_{N_2} , Y_{CH_4} , and Y_{O_2} . The values of Y_{CH_4} and Y_{O_2} can be calculated using the equations:

$$Y_{CH_4} = \frac{n_{CH_4}^0}{n_{CH_4}^0 + n_{O_2}^0 + n_{N_2}} \tag{11}$$

$$Y_{O_2} = \frac{n_{O_2}^0}{n_{CH_4}^0 + n_{O_2}^0 + n_{N_2}} \quad (12)$$

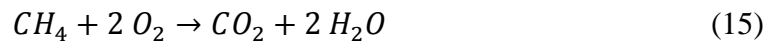
For example:

$$Y_{CH_4} = \frac{1 \text{ mol } CH_4}{1 \text{ mol } CH_4 + 19 \text{ mol } O_2 + 5 \text{ mol } N_2} \Rightarrow Y_{CH_4} = 0.04 \quad (13)$$

$$Y_{O_2} = \frac{19 \text{ mol } O_2}{1 \text{ mol } CH_4 + 19 \text{ mol } O_2 + 5 \text{ mol } N_2} \Rightarrow Y_{O_2} = 0.76 \quad (14)$$

The values of Y_{CH_4} and Y_{O_2} for every ratio of methane and oxygen for every n_{N_2} value are included in Section 3 of the Appendix. While these revised mole fractions do not have to be calculated at this particular point in the process because they won't be used until much later, it is convenient to calculate all the mole fractions at the same time.

The next step is to calculate the limiting reagent for each mole fraction using the initial moles of methane and oxygen and the molar ratios from the chemical equation. The chemical equation of this combustion reaction is given by:



The limiting reagent for the example being performed thus far can be calculated as follows:

$$1 \text{ mol } CH_4 \times \frac{2 \text{ mol } O_2}{1 \text{ mol } CH_4} = 2 \text{ mol } O_2 \quad (16)$$

$$2 \text{ mol} < 19 \text{ mol} \quad (17)$$

The amount of methane available will react with less oxygen than is available in this particular example, resulting in leftover oxygen while all the methane is combusted. This means that for this example, methane is the limiting reactant. As the amount of methane present is fixed at one mole it can be determined whether methane is the limiting reagent (if the full one mole of methane is used), or oxygen is the limiting reagent (if less than one mole of methane is combusted). Once the limiting reagent is determined, the amount of excess reagent leftover after

the combustion must be calculated. This can be done using the following equation, with n_i = the moles of the excess reagent leftover at the end of the reaction:

$$n^0_{\text{excess reagent}} - \left(n^0_{\text{limiting reagent}} \times \frac{\text{molar ratio of excess reagent}}{\text{molar ratio of limiting reagent}} \right) = n_{\text{excess reagent}}$$

Thus for our example the above equation becomes:

$$19 \text{ mols } O_2 - \left(1 \text{ mol } CH_4 \times \frac{2 \text{ mols } O_2}{1 \text{ mol } CH_4} \right) = 17 \text{ mols } O_2 \text{ remaining} \quad (18)$$

After the limiting reagent is determined, the moles of each product can be calculated using the following equation:

$$n^0_{\text{limiting reagent}} \times \frac{\text{molar ratio of product}}{\text{molar ratio of limiting reagent}} = n_{\text{product}} \quad (19)$$

For the example, the amount of CO_2 and H_2O produced would be:

$$1 \text{ mol } CH_4 \times \frac{1 \text{ mol } CO_2}{1 \text{ mol } CH_4} = 1 \text{ mol } CO_2 \quad (20)$$

$$1 \text{ mol } CH_4 \times \frac{2 \text{ mol } H_2O}{1 \text{ mol } CH_4} = 2 \text{ mol } H_2O \quad (21)$$

The results of all of these calculations (leftover moles of the excess reagent and produced moles for both CO_2 and H_2O) can be found in Section 4 of the Appendix. Because N_2 does not participate in the combustion, the moles of N_2 present are constant. Since we are considering an adiabatic reaction, all the heat from the combustion reaction goes into heating the mixture of products and reactants. The next step is to calculate the amount of heat produced by the reaction. This is done using the following equation:

$$(n^0_{CH_4} - n_{CH_4}) \Delta H_c = \text{released heat} \quad (22)$$

In our example the energy released is given by:

$$\frac{(1 \text{ mol} - 0 \text{ mol}) 802.3 \text{ kJ}}{\text{mol}} = 802.3 \text{ kJ} \quad (23)$$

The calculated energies produced for each ratio of methane to oxygen are given in Section 5 of the appendix. This value is then set equal to equation (3) which gives the amount of energy that goes into heating the mixture of products and leftover reactant gasses. Thus for our prolonged example this becomes:

$$\begin{aligned} & \left(0 \int_{25}^{T_A} (0.034 + 2.50 \times 10^{-6} T) dT \right) + \left(17 \int_{25}^{T_A} (0.03 + 3.00 \times 10^{-6} T) dT \right) \\ & + \left(1 \int_{25}^{T_A} (0.04 + 9.70 \times 10^{-6} T) dT \right) + \left(2 \int_{25}^{T_A} (0.033 + 5.50 \times 10^{-6} T) dT \right) \\ & = 802.3 \text{ kJ/mol} \end{aligned} \quad (24)$$

Now evaluating the integrals in (24) yields:

$$4.135 \times 10^{-5} T_A^2 + 0.801 T_A - 822.351 \text{ kJ/mol} = 0 \quad (25)$$

We rewrite (25) as:

$$a T_A^2 + b T_A + c = 0 \quad (26)$$

As (26) is a quadratic polynomial, we can solve for T_A via the quadratic equation. The values for a , b , and c for each mole fraction of methane and oxygen at all Y_{N_2} values are listed in Section 8 of Appendix A. For our example this is done as follows:

$$\begin{aligned} T_A &= \frac{-0.801 \pm \sqrt{(0.801)^2 - 4(4.135 \times 10^{-5})(-822.3365)}}{2(4.135 \times 10^{-5})} \\ T_A &= \frac{-0.801 \pm \sqrt{0.6552}}{8.27 \times 10^{-5}} \end{aligned} \quad (27)$$

$$T_A(\text{plus}) = 977.33, \quad T_A(\text{minus}) = -20348.5$$

Since the value $T_A(\text{minus})$ is not feasible we determine the legitimate T_A value is given by $T_A(\text{plus}) = 977.33$. In this case, with a mole ratio of methane to oxygen of $Y' = 0.05$ and $Y_{N_2} = 0.2$, the T_A value is 977.33. The values obtained by both adding and subtracting the square root for every mole fraction at all Y_{N_2} values are included in Section 8 of Appendix A.

Based on the values obtained for the adiabatic flame temperature, the following graph was produced for the mole fraction of methane at a constant Y_{N_2} value.

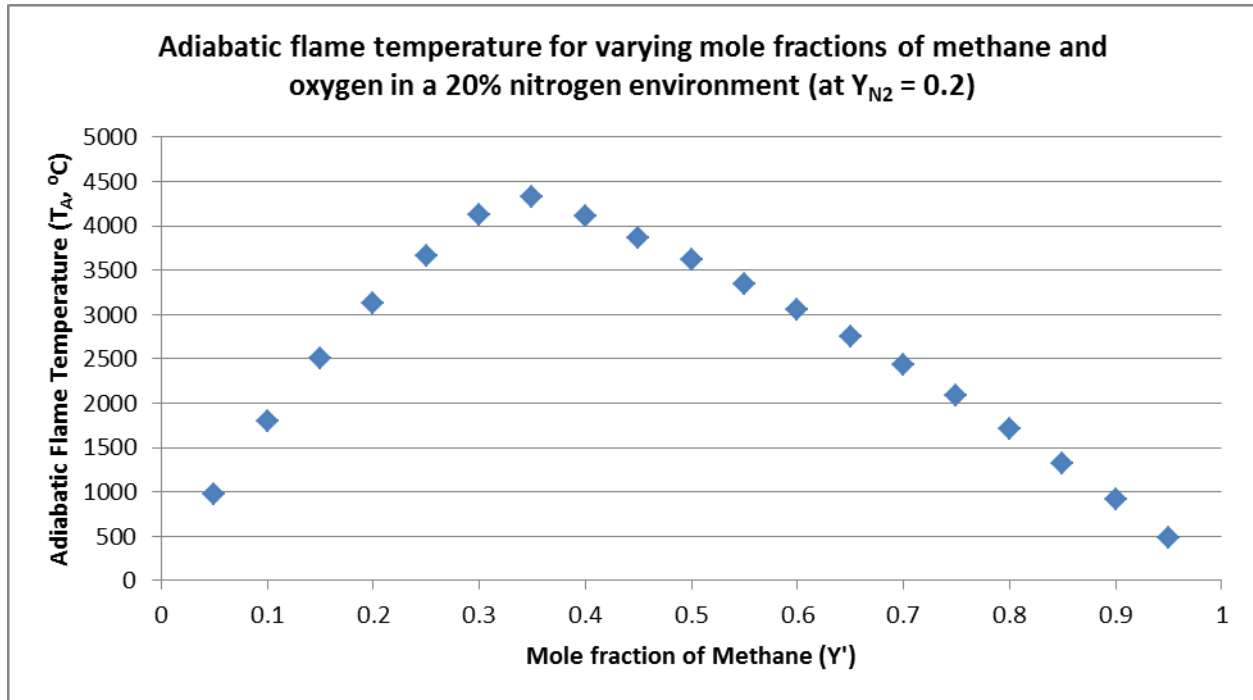


Figure 1: Adiabatic flame temperature for varying mole fractions of methane and oxygen in a 20% nitrogen environment.

The graphs produced for the adiabatic flame temperature at each mole fraction of methane at each Y_{N_2} can be found in Section 10 of the appendix. Additionally, all the data points were combined to create a graph comparing the adiabatic flame temperature trend in each different nitrogen environment.

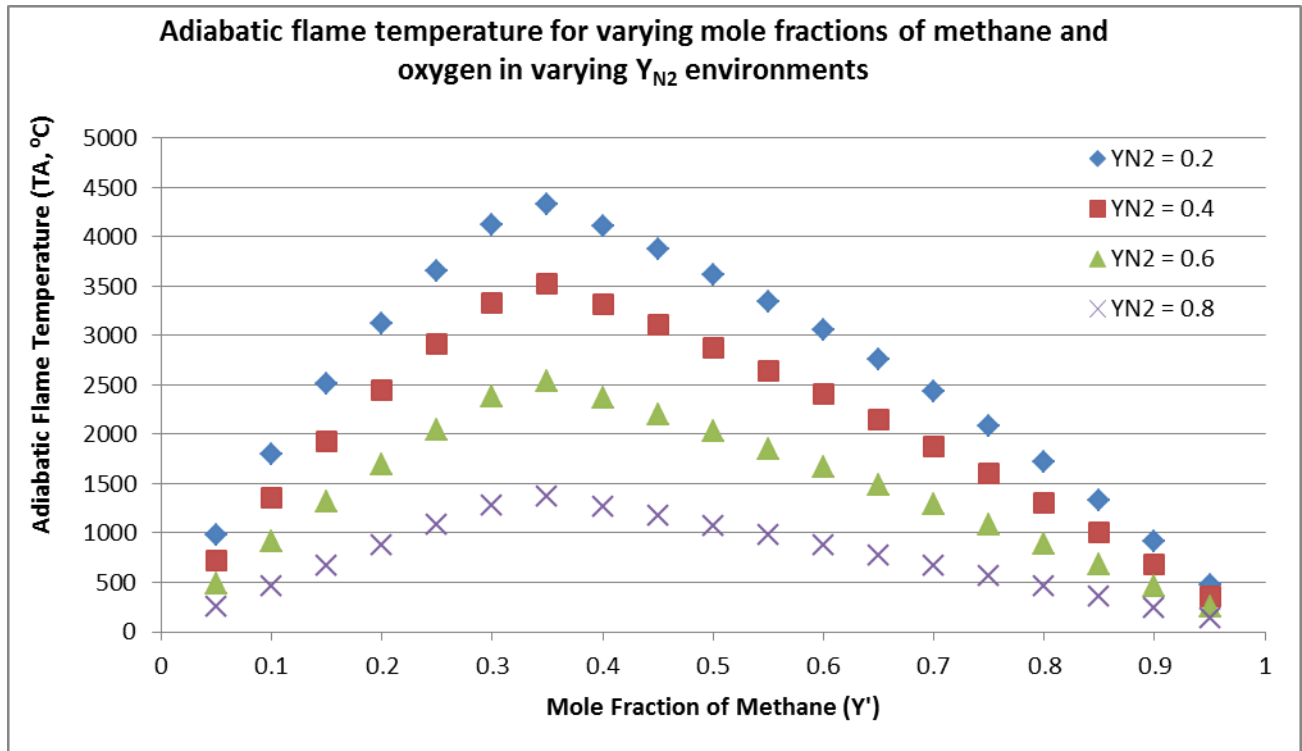


Figure 2: Mole fraction of methane Y_{N_2} .

Lastly, a ternary chart was produced to compare the adiabatic flame temperature at each Y_{CH_4} , Y_{O_2} , and Y_{N_2} evaluated. Colors were assigned to ranges of $500^{\circ}C$, and each individual $(Y_{CH_4}, Y_{O_2}, Y_{N_2})$ point was classified in one of those ranges. The points were all graphed in their respective color, and the rest of the graph was filled in by extrapolation using a ruler. The lines of different colors show similar adiabatic flame temperatures across different Y_{N_2} values.

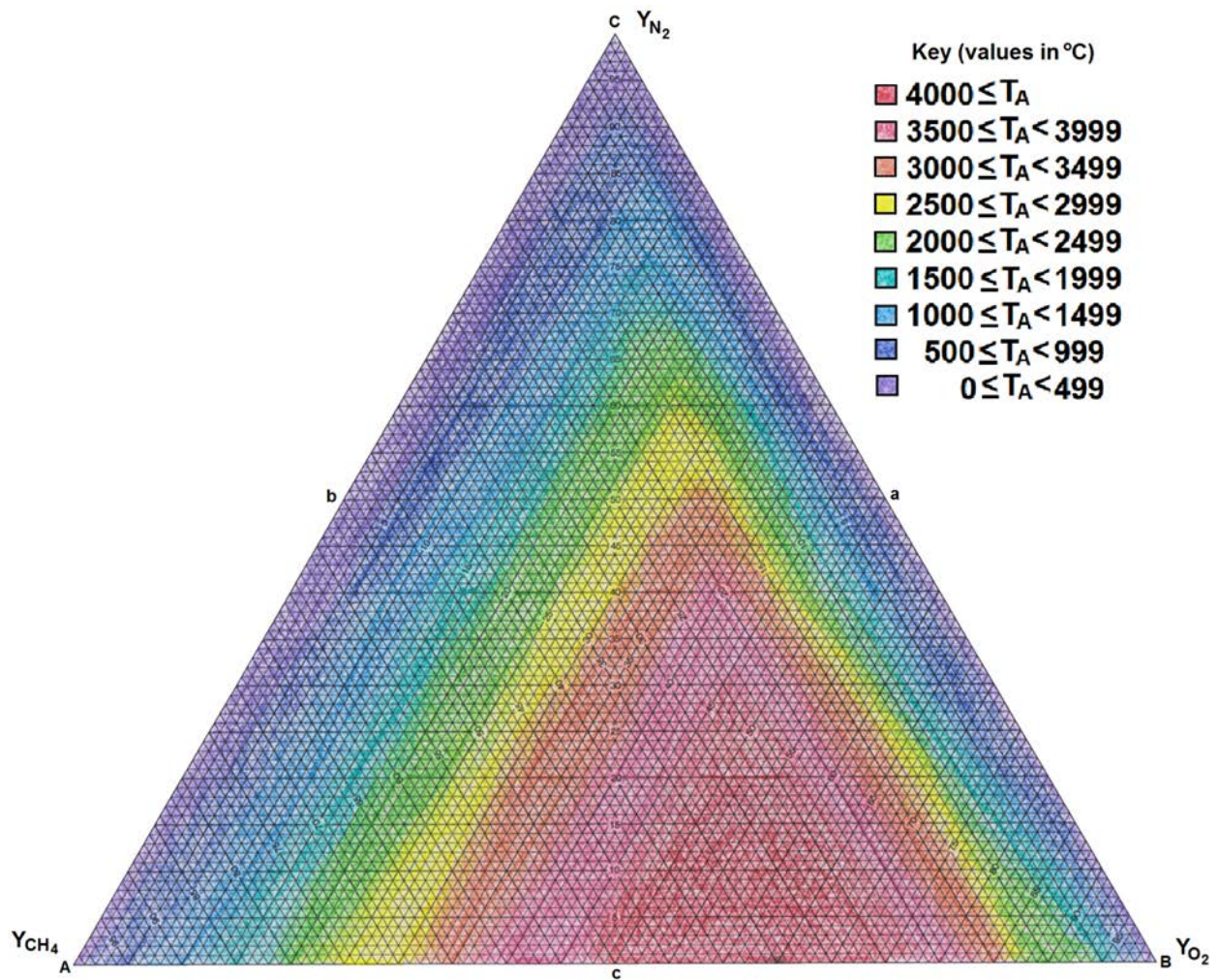


Figure 3: Ternary Chart modeling comparing the adiabatic flame temperature at each Y_{CH_4} , Y_{O_2} , and Y_{N_2} evaluated.

DISCUSSION

Unsurprisingly, the higher the concentration of the diluent gas (N_2), the lower the adiabatic flame temperature for that mole fraction of methane. This is expected because the diluent gas does not contribute any energy to the reaction and just acts as a drain on the adiabatic flame temperature. This is apparent from the overlaid graphs at each Y_{N_2} , and also from the ternary diagram. Additionally, for each mole fraction of methane, $Y' = 0.35$ was still the mole

fraction with the highest adiabatic flame temperature. While the ideal mole fraction was also apparent in the last project, this project confirms that the addition of a diluent does not change the ideal molar ratio of combustion of two reactants.

Additionally, based on the overlay of graphs and the ternary chart, certain flame temperatures can be produced at multiple Y_{N_2} values by changing the amount of oxygen present in the system. This could be useful in planning a combustion reaction to account for certain amounts of diluents entering the system while still producing the desired temperature.

CONCLUSION AND RECOMMENDATIONS

The highest adiabatic flame temperature occurring at each respective mole fraction of nitrogen decreases as more nitrogen is added. This makes sense, because adding extra diluent provides material that will still draw heat from the resulting combustion, while also reducing the amount of reactants and thus the amount of energy produced by the reaction.

Additionally, the highest adiabatic flame temperature evaluated for every mole fraction of nitrogen occurs when the mole fraction of methane without respect to nitrogen equals 0.35. This shows that the addition of a diluents gas does not affect the ideal molar ratio for the combustion reaction. This can be seen on the overlaid graph that shows the curve of the adiabatic flame temperature for each constant mole fraction of nitrogen present.

The ternary diagram and overlaid graph both show that the same adiabatic flame temperature can be produced at different mole fractions of nitrogen. This leads to the conclusion that certain amounts of diluents can be allowed into the combustion system alongside the reactants, resulting in the same flame temperature provided the mole fraction of methane is

adjusted accordingly. For example, an adiabatic flame temperature of 2000°C can be produced at $Y_{N_2} = 0.2, 0.4, 0.6$ at different mole fractions of methane, approximately $Y' = 0.1, 0.15,$ and 0.25 respectively. This can be useful in accounting for diluents in the feed stream in the reactor while still producing the same heat output.

For a slightly future project, all the mole fractions of methane, oxygen, and nitrogen that produce a particular adiabatic flame temperature could be evaluated to produce a list of conditions that will still produce the ideal temperature for the production of some material. To further explore this reactive combination of methane and oxygen, the hindrance factors of different diluents could be compared (for example, using a noble gas as the diluent as compared to nitrogen) at constant mole fractions (for example, $Y' = 0.33,$ and $Y_{diluent} = 0.2$) to see which diluents have the greatest affect on the maximum adiabatic flame temperature.

NOMENCLATURE

Symbol	Description	Units
Y'	Mole fraction (nitrogen free)	
Y_i	Mole fraction with respect to the amount of nitrogen present	
n_i^0	Moles present before combustion	mol
n_i	Moles present after combustion	mol
ΔH_c	Energy produced from the combustion of methane	kJ/mol
Cp_i	Heat capacity	kJ/(mol* $^{\circ}$ C)
A_i	constant	kJ/(mol* $^{\circ}$ C)
B_i	constant	kJ/(mol*($^{\circ}$ C) 2)
T	Temperature	$^{\circ}$ C
a	T_A^2 coefficient in the quadratic equation	
b	T_A coefficient in the quadratic equation	
c	Constant in the quadratic equation	
T_A	Adiabatic flame temperature	$^{\circ}$ C

REFERENCES

Campbell, Scott. Interview. Rebeca Pupo. 2012.

Crowl, Daniel A. Understanding Explosions 1. New York City: Center for Chemical Process Safety, 2010.

Larson, Ron, Robert Hostetler and Bruce Edwards. Calculus. 8th Edition. Boston, MA: Houghton Mifflin Company, 2005.

Pupo, Rebeca. "Adiabatic Flame Temperature for Combustion of Methane." Undergraduate Journal of Mathematical Modeling (2011).

APPENDICES

APPENDIX A – TABLES

Section 1: Initial moles of CH₄ and O₂ for each mole fraction on a nitrogen-free basis.

Y'	$n_{\text{CH}_4}^0$ (mol)	$n_{\text{O}_2}^0$ (mol)
0.05	1.00	19.00
0.10	1.00	9.00
0.15	1.00	5.67
0.20	1.00	4.00
0.25	1.00	3.00
0.30	1.00	2.33
0.35	1.00	1.86
0.40	1.00	1.50
0.45	1.00	1.22
0.50	1.00	1.00
0.55	1.00	0.82
0.60	1.00	0.67
0.65	1.00	0.54
0.70	1.00	0.43
0.75	1.00	0.33
0.80	1.00	0.25
0.85	1.00	0.18
0.90	1.00	0.11
0.95	1.00	0.05

Section 2: Moles of N₂ present along with each mole fraction of methane and oxygen at variable Y_{N_2} values.

Moles of N ₂ at Y_{N_2}				
Y'	n_{N_2} at $Y_{\text{N}_2} = 0.2$	n_{N_2} at $Y_{\text{N}_2} = 0.4$	n_{N_2} at $Y_{\text{N}_2} = 0.6$	n_{N_2} at $Y_{\text{N}_2} = 0.8$
0.05	5.00	13.33	30.00	80.00
0.10	2.50	6.67	15.00	40.00
0.15	1.67	4.44	10.00	26.67
0.20	1.25	3.33	7.50	20.00
0.25	1.00	2.67	6.00	16.00
0.30	0.83	2.22	5.00	13.33
0.35	0.71	1.90	4.29	11.43
0.40	0.63	1.67	3.75	10.00
0.45	0.56	1.48	3.33	8.89
0.50	0.50	1.33	3.00	8.00
0.55	0.45	1.21	2.73	7.27
0.60	0.42	1.11	2.50	6.67
0.65	0.38	1.03	2.31	6.15
0.70	0.36	0.95	2.14	5.71
0.75	0.33	0.89	2.00	5.33
0.80	0.32	0.83	1.88	5.00
0.85	0.29	0.78	1.76	4.71
0.90	0.28	0.74	1.67	4.44
0.95	0.26	0.70	1.58	4.21

Section 3: Mole fractions of CH₄ and O₂ respectively with respect to the moles of N₂ present.

Mole fractions of CH ₄ at Y _{N₂}				
Y'	Y _{CH₄} at Y _{N₂} = 0.2	Y _{CH₄} at Y _{N₂} = 0.4	Y _{CH₄} at Y _{N₂} = 0.6	Y _{CH₄} at Y _{N₂} = 0.8
0.05	0.04	0.03	0.02	0.01
0.10	0.08	0.06	0.04	0.02
0.15	0.12	0.09	0.06	0.03
0.20	0.16	0.12	0.08	0.04
0.25	0.20	0.15	0.10	0.05
0.30	0.24	0.18	0.12	0.06
0.35	0.28	0.21	0.14	0.07
0.40	0.32	0.24	0.16	0.08
0.45	0.36	0.27	0.18	0.09
0.50	0.40	0.30	0.20	0.10
0.55	0.44	0.33	0.22	0.11
0.60	0.48	0.36	0.24	0.12
0.65	0.52	0.39	0.26	0.13
0.70	0.56	0.42	0.28	0.14
0.75	0.60	0.45	0.30	0.15
0.80	0.64	0.48	0.32	0.16
0.85	0.68	0.51	0.34	0.17
0.90	0.72	0.54	0.36	0.18
0.95	0.76	0.57	0.38	0.19

Mole fractions of O ₂ (Y _{O₂}) at Y _{N₂}				
Y'	Y _{O₂} at Y _{N₂} = 0.2	Y _{O₂} at Y _{N₂} = 0.4	Y _{O₂} at Y _{N₂} = 0.6	Y _{O₂} at Y _{N₂} = 0.8
0.05	0.76	0.57	0.38	0.19
0.10	0.72	0.54	0.36	0.18
0.15	0.68	0.51	0.34	0.17
0.20	0.64	0.48	0.32	0.16
0.25	0.60	0.45	0.30	0.15
0.30	0.56	0.42	0.28	0.14
0.35	0.52	0.39	0.26	0.13
0.40	0.48	0.36	0.24	0.12
0.45	0.44	0.33	0.22	0.11
0.50	0.40	0.30	0.20	0.10
0.55	0.36	0.27	0.18	0.09
0.60	0.32	0.24	0.16	0.08
0.65	0.28	0.21	0.14	0.07
0.70	0.24	0.18	0.12	0.06
0.75	0.20	0.15	0.10	0.05
0.80	0.16	0.12	0.08	0.04
0.85	0.12	0.09	0.06	0.03
0.90	0.08	0.06	0.04	0.02
0.95	0.04	0.03	0.02	0.01

Section 4: The moles of each species present after the combustion reaction has taken place with respect to the mole fraction of methane.

Leftover/produced moles of each species				
Y'	n_{CH_4} (mol)	n_{O_2} (mol)	n_{CO_2} (mol)	$n_{\text{H}_2\text{O}}$ (mol)
0.05	0.00	17.00	1.00	2.00
0.10	0.00	7.00	1.00	2.00
0.15	0.00	3.67	1.00	2.00
0.20	0.00	2.00	1.00	2.00
0.25	0.00	1.00	1.00	2.00
0.30	0.00	0.33	1.00	2.00
0.35	0.07	0.00	0.93	1.86
0.40	0.25	0.00	0.75	1.50
0.45	0.39	0.00	0.61	1.22
0.50	0.50	0.00	0.50	1.00
0.55	0.59	0.00	0.41	0.82
0.60	0.67	0.00	0.33	0.67
0.65	0.73	0.00	0.27	0.54
0.70	0.79	0.00	0.21	0.43
0.75	0.83	0.00	0.17	0.33
0.80	0.88	0.00	0.13	0.25
0.85	0.91	0.00	0.09	0.18
0.90	0.94	0.00	0.06	0.11
0.95	0.97	0.00	0.03	0.05

Section 5: Energy produced from the combustion reaction for each mole fraction of CH_4 and O_2 .

Energy Liberated from Combustion	
Y'	$(n_{\text{CH}_4}^0 - n_{\text{CH}_4})\Delta H$ (kJ)
0.05	802.30
0.10	802.30
0.15	802.30
0.20	802.30
0.25	802.30
0.30	802.30
0.35	744.99
0.40	601.73
0.45	490.29
0.50	401.15
0.55	328.21
0.60	267.43
0.65	216.00
0.70	171.92
0.75	133.72
0.80	100.29
0.85	70.79
0.90	44.57
0.95	21.11

Section 6: The values for A and B for each of the species present.

Gas	A	B
CH_4	0.034	2.50E-06
O_2	0.03	3.00E-06
CO_2	0.04	9.70E-06
H_2O	0.033	5.50E-06
N_2	0.037	2.20E-06

Section 7: Quadratic coefficients A, B, and C for each mole fraction of CH₄ and O₂.

Quadratic Equation Coefficients for $Y_{N_2} = 0.2$			
Y'	a	b	C
0.05	41.35 E-06	0.801	-822.34
0.10	23.60 E-06	0.409	-812.52
0.15	17.68 E-06	0.278	-809.25
0.20	14.73 E-06	0.212	-807.61
0.25	12.95 E-06	0.173	-806.63
0.30	11.77 E-06	0.147	-805.98
0.35	10.49 E-06	0.127	-748.18
0.40	8.76 E-06	0.111	-604.51
0.45	7.42 E-06	0.099	-492.76
0.50	6.35 E-06	0.089	-403.37
0.55	5.47 E-06	0.080	-330.22
0.60	4.74 E-06	0.073	-269.27
0.65	4.12 E-06	0.068	-217.70
0.70	3.59 E-06	0.063	-173.49
0.75	3.13 E-06	0.058	-135.18
0.80	2.73 E-06	0.055	-101.65
0.85	2.38 E-06	0.051	-72.07
0.90	2.06 E-06	0.048	-45.78
0.95	1.78 E-06	0.046	-22.26

Quadratic Equation Coefficients for $Y_{N_2} = 0.4$			
Y'	a	b	c
0.05	50.52 E-06	1.110	-830.05
0.10	28.18 E-06	0.563	-816.38
0.15	20.74 E-06	0.380	-811.82
0.20	17.02 E-06	0.289	-809.54
0.25	14.78 E-06	0.235	-808.17
0.30	13.29 E-06	0.198	-807.26
0.35	11.80 E-06	0.171	-749.28
0.40	9.91 E-06	0.150	-605.47
0.45	8.44 E-06	0.133	-493.62
0.50	7.27 E-06	0.119	-404.14
0.55	6.31 E-06	0.108	-330.93
0.60	5.51 E-06	0.099	-269.91
0.65	4.83 E-06	0.091	-218.29
0.70	4.25 E-06	0.085	-174.04
0.75	3.74 E-06	0.079	-135.69
0.80	3.30 E-06	0.074	-102.14
0.85	2.92 E-06	0.069	-72.53
0.90	2.57 E-06	0.065	-46.21
0.95	2.26 E-06	0.062	-22.66

Quadratic Equation Coefficients for $Y_{N_2} = 0.6$			
Y'	a	b	c
0.05	68.85 E-06	1.726	-845.48
0.10	37.35 E-06	0.871	-824.09
0.15	26.85 E-06	0.586	-816.96
0.20	21.60 E-06	0.444	-813.40
0.25	18.45 E-06	0.358	-811.26
0.30	16.35 E-06	0.301	-809.83
0.35	14.41 E-06	0.259	-751.49
0.40	12.20 E-06	0.227	-607.40
0.45	10.478 E-06	0.201	-495.33
0.50	9.10 E-06	0.181	-405.68
0.55	7.97 E-06	0.164	-332.33
0.60	7.03 E-06	0.151	-271.20
0.65	6.24 E-06	0.139	-219.48
0.70	5.56 E-06	0.129	-175.14
0.75	4.97 E-06	0.120	-136.72
0.80	4.45 E-06	0.112	-103.10
0.85	3.99 E-06	0.106	-73.43
0.90	3.59 E-06	0.100	-47.07
0.95	3.23 E-06	0.094	-23.47

Quadratic Equation Coefficients for $Y_{N_2} = 0.8$			
Y'	a	b	c
0.05	123.85 E-06	3.576	-891.76
0.10	64.85 E-06	1.796	-847.23
0.15	45.18 E-06	1.203	-832.39
0.20	35.35 E-06	0.906	-824.97
0.25	29.45 E-06	0.728	-820.52
0.30	25.52 E-06	0.609	-817.55
0.35	22.27 E-06	0.524	-758.10
0.40	19.08 E-06	0.458	-613.19
0.45	16.59 E-06	0.407	-500.48
0.50	14.60 E-06	0.366	-410.31
0.55	12.97 E-06	0.333	-336.54
0.60	11.62 E-06	0.305	-275.06
0.65	10.47 E-06	0.281	-223.04
0.70	9.49 E-06	0.261	-178.45
0.75	8.63 E-06	0.243	-139.81
0.80	7.89 E-06	0.228	-105.99
0.85	7.23 E-06	0.214	-76.16
0.90	6.64 E-06	0.202	-49.64
0.95	6.12 E-06	0.192	-25.91

Section 8: T_A values obtained for each mole fraction at different Y_{N_2} values.

T_A at $Y_{N_2} = 0.2$		
Y'	Plus ($^{\circ}\text{C}$)	Minus (discard)
0.05	977.3	-20348.5
0.10	1801.5	-19110.9
0.15	2512.5	-18214.6
0.20	3126.8	-17541
0.25	3659.9	-17019
0.30	4125.3	-16604.1
0.35	4332.0	-16471
0.40	4108.7	-16790.6
0.45	3871.2	-17149.7
0.50	3618.4	-17555.4
0.55	3349.1	-18016.9
0.60	3062.1	-18545.4
0.65	2756.4	-19155.6
0.70	2430.7	-19866
0.75	2084.0	-20701
0.80	1715.7	-21692.8
0.85	1325.3	-22884.7
0.90	912.7	-24335.9
0.95	478.8	-26129.7

T_A at $Y_{N_2} = 0.4$		
Y'	Plus ($^{\circ}\text{C}$)	Minus (discard)
0.05	724.3	-22684.1
0.10	1358.5	-21323.0
0.15	1930.7	-20275.2
0.20	2446.1	-19449.0
0.25	2910.3	-18784.1
0.30	3329.2	-18239.3
0.35	3520.2	-18045.8
0.40	3317.1	-18422.2
0.45	3104.2	-18839.2
0.50	2881.1	-19303.2
0.55	2647.4	-19821.9
0.60	2402.7	-20404.7
0.65	2146.5	-21063.1
0.70	1878.6	-21811.3
0.75	1598.7	-22667
0.80	1306.9	-23652.4
0.85	1003.2	-24796.1
0.90	687.9	-26134.6
0.95	361.6	-27716.1

T_A at Y_{N2} = 0.6		
Y'	Plus (°C)	Minus (discard)
0.05	480.6	-25549.6
0.10	910.5882	-24230.5
0.15	1314.914	-23139.9
0.20	1694.244	-22226.7
0.25	2049.595	-21453.4
0.30	2382.222	-20792
0.35	2538.629	-20536.6
0.40	2375.191	-20961.3
0.45	2206.822	-21422.1
0.50	2033.443	-21923.6
0.55	1854.994	-22470.7
0.60	1671.437	-23069.5
0.65	1482.759	-23726.9
0.70	1288.977	-24450.9
0.75	1090.144	-25251.2
0.80	886.3507	-26139.2
0.85	677.7309	-27128.4
0.90	464.4672	-28235.4
0.95	246.7939	-29480.1

T_A at Y_{N2} = 0.8		
Y'	Plus (°C)	Minus (discard)
0.05	247.2567	-29120.9
0.1	463.9613	-28158.6
0.15	675.0038	-27292.5
0.2	880.3255	-26509.7
0.25	1079.908	-25799.8
0.3	1273.767	-25153.6
0.35	1367.964	-24883
0.4	1271.502	-25282
0.45	1173.833	-25701.6
0.5	1074.967	-26143.5
0.55	974.92	-26609.1
0.6	873.7074	-27100.4
0.65	771.3488	-27619.3
0.7	667.8664	-28167.9
0.75	563.2854	-28748.6
0.8	457.634	-29364.1
0.85	350.9436	-30017.3
0.9	243.2486	-30711.5
0.95	134.5871	-31450.2

APPENDIX B - GRAPHS

Section 9: Graphs of the mole fraction of methane compared to the adiabatic flame temperature of that mixture at constant Y_{N_2} .

