Combustion Characteristics of Propane: Effect of equivalence ratio on flame structure and color, liftoff and flashback phenomena, flame propagation speed, detonation, and critical diameter

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Abstract:
Combustion is ubiquitous in everyday life, and an understanding of flame behavior is important in understanding this vital energy source. A propane Bunsen burner combustion training apparatus was utilized to record the effect of equivalence ratio on flame shape, color, and structure of a flame, to determine liftoff conditions, to observe blowback and detonation phenomena, determine laminar flame propagation speed, and to observe the effect of sub-critical diameter mesh on flame behavior. Luminosity was observed to be highest for soot producing, diffusion flame. Increasing airflow caused a blue glow that intensified with decreasing equivalence ratio due to excited C₂, CH, and OH radicals. The flame stabilizer caused a 4.5% increase in airflow capability. Laminar flame propagation velocity was determined to be approximately 106 cm/s.

Introduction:
Combustion is ubiquitous in everyday life. In 2007, approximately 85% of all energy used in the United States came from combustion sources [1]. Combustion is useful primarily because of the heat release that it generates, which comes from the flame [2]. An understanding of the factors influencing flame is important to understanding and optimizing energy use and generation [1]. The goal of this experiment is to understand the effect of equivalence ratio on flame shape, color, and structure of a propane Bunsen burner flame, to determine liftoff conditions, to observe blowback and detonation phenomena, determine laminar propane flame propagation speed, and observe the effect of sub-critical diameter mesh on flame behavior utilizing a Bunsen burner combustion training apparatus with propane fuel.

Theory:
Equivalence Ratio and Flammability Limits
A flame is a zone of finite thickness where rapid chemical reactions occur [1]. The characteristics of a flame vary significantly with the amount of fuel present relative to the amount of air, or oxidizer, available to burn it [2]. The balanced equation for the complete combustion of hydrocarbon is shown by equation 1.

\[
C_xH_y + a(O_2 + 3.76 N_2) \rightarrow xCO_2 + (y/2)O_2 + 3.76aN_2
\]

\(a = x + y/4\)

Equation 1: Stoichiometric Combustion of a hydrocarbon [1]
From the balanced equation for complete combustion, stoichiometric air to fuel ratio on a mass basis can be calculated then compared to actual air to fuel ratio. This comparison is known as equivalence ratio and is calculated on a mass basis using equation 2.

\[\frac{(A/F)_{stoch}}{MW_{fuel}} = \frac{4.76a}{MW_{air}}\]

And \(\frac{(A/F)}{MW_{fuel}} = \frac{n_{air}}{n_{fuel}}\)

Then \(\phi = \frac{(A/F)_{stoch}}{MW_{air}}\)

Equation 2: Equivalence Ratio Calculation [1]
Where \((A/F)_{stoch}\) is the stoichiometric air to fuel ratio, \(a\) is the coefficient for moles of air from equation 1, \(MW\) is molecular weight of air and fuel in g/mol, \((A/F)\) is the actual air to fuel ratio, \(n_{air}\) is the number of moles of air, \(n_{fuel}\) is the number of moles of fuel. Equivalence ratio \(\Phi\) is calculated by dividing stoichiometric air to fuel ratio by the actual air to fuel ratio. An equivalence ratio of 1 denotes stoichiometric combustion, and equivalence of greater that one means that the combustion is fuel rich (not enough air present to burn the quantity of fuel completely), and an equivalence ratio of less than one means that that combustion is fuel lean (there is more air than required to burn the quantity of fuel present) [1-2].
Flames will only propagate if the relative amounts of fuel and air present are within the particular fuels’ flammability limit [2]. Flame will not propagate if equivalence ratio is too high (upper limit) or too low (lower limit) [2]. At the upper limit, the fuel dilutes the oxygen required for combustion to occur [1]. Near the lean limit, heat is lost to surrounding air such that temperature cannot reach a level that sustains combustion [1]. Upper (rich) flammability limit for propane is 2.83 and the lower (lean) flammability limit is 0.51 [1].

**Flame Characteristics**

Between flammability limits, flame characteristics vary significantly. A Bunsen burner flame is a pre-mixed combustion system when air intake ports are open [1]. Propane and air are allowed to fully mix before reaching the flame front [1]. Lean laminar premixed flames are characterized by their blue color, which results from excited CH radicals [3]. Equivalence ratios closer to one result in blue-green flame due to excited C₂[3]. The OH radical also contributes to the visible radiation emitted by both fuel lean and fuel rich premixed flames [1][3]. A diffusion flame results if airflow is cut off from the Bunsen burner. In a diffusion flame, soot particles form via a complex chemical process explained in question 5 [1]. Soot, due to particle size, interacts with and scatters infrared light[4]. The human eye perceives this radiation as an orange-white glow[1].

The structure of a laminar premixed Bunsen flame is characterized by an inner conical pre-mixed flame and an outer diffusion flame, which is the result of carbon monoxide and hydrogen products coming into contact with ambient air [1]. Premixed Bunsen flames, since reactants enter from the tube, are conical due to the velocity profile of the air-fuel mixture, but also because the velocity vector normal to the flame surface must equal laminar burning velocity Sₗ [1]. If laminar-burning velocity is high, a narrow flame results and visa versa. This is shown by equation 3.

\[ S_\ell = v_e \sin \alpha \]

**Equation 3: Bunsen burner flame angle [1]**

Where \( S_\ell \) equals flame speed in cm/s, \( v_e \) equals velocity of incoming fuel and air mixture in cm/s, and \( \alpha \) equals Bunsen flame angle.

Laminar diffusion flames differ from laminar pre-mixed flames in their mode of mass transfer of reactants to the combustion zone[1]. In a diffusion flame, air diffuses from the outside of the flame inward, while fuel diffuses from the inside outwards[1]. The surface of a laminar diffusion flame exists where air and fuel mix at stoichiometric proportions[1].

**Flame Propagation and Detonation**

A flame can be described as a self-sustaining propagation of localized combustion zone at subsonic velocities [1]. The speed at which a flame propagates depends on many factors, but when allowed to freely propagate, the flame front approaches flame speed \( S_\ell \) [1]. A flame only exists if the reactants enter the flame with a velocity normal to the flame front that is equal to the flame speed [1]. When reactants are stationary, the flame propagation speed equals the velocity at which reactants are entering the flame front. For a laminar flame, flame speed is heavily dependent on equivalence ratio, fuel type, temperature, and diluent present [1]. Empirical methods have been employed to determine the laminar flame speeds of a variety of fuels at 298 K, equivalence ratio of 1, and pressure of 1 atm[1]. Laminar flame speed for propane has been experimentally determined to be 44 centimeters per second at an equivalence ration of 1, at room temperature and 1 atm [1]. Maximum laminar flame propagation speed typically occurs at an equivalence ratio of one[2].

A detonation is a shock wave supported by a zone of rapid chemical reaction [1-2]. When a fuel-air mixture is ignited at the closed end of a tube that is open at the other end, the flame that results is accelerated by the pressure wave that the expanded gases between the flame and bottom of the tube create[1-2]. This acceleration leads to the formation of a shockwave propagating faster than the speed of sound[1]. This rapid compression causes
local temperatures high enough to sustain combustion [1-2]. Detonation waves travel at supersonic speeds ranging from 1 to 4 kilometers per second [2]. Detonation speed is equal to the velocity at which reactants enter the flame front, which is the same principal as flame propagation [1]. Detonation velocity can be calculated using equation 4. Detonation velocity depends fundamentally on the specific heats before and after the reaction occurs, equivalence ratio, as well as on temperature and heat release of the fuel used [1].

\[
v_D = \left[2(\gamma + 1)\gamma R_2\left(\frac{c_{p,1}}{c_{p,2}} T_1 + \frac{q}{c_{p,2}}\right)\right]^{1/2} \text{ and } T_2 = \frac{2\gamma^2}{\gamma + 1}\left(\frac{c_{p,1}}{c_{p,2}} T_1 + \frac{q}{c_{p,2}}\right)
\]

**Equation 4: Flame detonation velocity [1]**

Where \(v_D\) is detonation velocity in meters per second, \(\gamma\) is the ratio of constant pressure specific heat over constant pressure heat capacity, \(T_1\) equals initial temperature in Kelvin, \(T_2\) equals final temperature in Kelvin, \(q\) equals heat release in kJ/kg, \(c_{p,1}\) and \(c_{p,2}\) are initial and final specific heats respectively in kJ/kg-K [1].

*Flashback, Liftoff, and Flashback Phenomena*

Flashback occurs when flame burning velocity exceeds flow velocity of species into the flame [2]. Low flow velocities of species into a flame cause the flame to move in the opposite direction of the flow[2]. When local flame speeds exceed local flow velocity, the flame propagates upstream through any opening greater than the flame’s quenching distance[1].

At low flow velocities, flame edge is close to the burner edge and is attached [2]. An attached flame is the result of low local flow velocity due to the boundary layer that develops at the tube wall [1-2]. At the tube wall surface, flow velocity of pre-mixes gases is zero[1]. Also, the tube absorbs heat from the flame locally[1]. The combination of low flow velocity and lower local temperature result in a low local laminar flame speed, which results in an attached flame [2]. If flow velocity is increased, flame angle will decrease by equation 3. This will pull the flame base away from the burner tip and into regions of increasing flow velocity and temperature until the liftoff point is reached[1]. At the liftoff point, the flame base detaches and stabilizes downstream[1]. Stabilizers are designed to reduce local flow velocities and promote flame attachment [2].

**Critical Diameter/ Quenching Distance**

A flame will propagate down an open tube or opening, but only if that opening is greater than the flame’s critical diameter under those conditions [2]. Quenching distance is a function of flame thickness and temperature gradient between flame and the walls of the opening[1]. When the diameter of the port becomes smaller than the quenching distance, sufficient mass flow cannot be obtained and heat transfer from flame front to the walls of the opening make it impossible to sustain a flame [2]. Quenching distance, or critical diameter for propane at an equivalence ratio 1 is 2 millimeters, while the absolute minimum quenching distance for propane at any equivalence ratio is 1.8 millimeters[1].

**Methods:**

Flame structure is influenced by many factors. The effect of varying equivalence ratios in a Bunsen burner flame was examined to determine how variation affected flame structure, detachment and stabilization phenomena, as well as blowback phenomena. Flame front velocity and detonation were also examined using a combustion trainer system.

To determine the effect of equivalence ratio on flame characteristics fuel flow to a Bunsen burner was set to 80 mL/min and pressure was recorded. Air flow was brought to 0mL/min and pressure was recorded. Fuel flow was held constant while air flow was increased in increments of 15 mL/minute until a 60mL/min air flow rate was achieved. Pressure readings were recorded at each condition and flame structure and color were recorded by taking photographs of the flame.
To determine liftoff conditions fuel flow was held at 80mL/min and air flow was increased until flame completely detached from the tube edge. Air flowrate was recorded and repeated in triplicate. This process was repeated without the hexagonal flame stabilized to determine the difference with and without the stabilizer.

To observe a blowback event, a glass Bunsen burner tube was used and fuel and air were brought to conditions that produced an unsteady flame. Fuel flow was cut off to observe propagation back into the tube.

To observe the effect of a mesh below quenching distance on the flame, wire mesh was placed about 2 inches over the flame to determine if the mesh allowed flame propagation below it.

To observe a detonation event, propane was allowed to fill a long glass tube loosely capped at the top. A spark gun was inserted into the bottom of the tube. Spark was ignited at the bottom of the tube and detonation event was observed.

To determine laminar flame propagation speed, propane was allowed to fill the same glass tube used in detonation observation and ignited via a match at the top. Flame propagation down the tube was observed and recorded on video for determination of laminar flame propagation speed.

**Results and Discussion:**

Varying equivalence ratio was shown to have a significant effect on flame shape, size, structure, and color as shown by figure 1. Soot formation in flame 1 caused a luminous orange flame. Increasing airflow caused a blue glow that intensified with decreasing equivalence ratio due to excited C\textsubscript{2}, CH, and OH radicals. In flames 4 and 5 the formation of two distinct flame zones was evident. The area marked “a” represents the premixed cone and the zone labeled “b” was the secondary diffusion flame. Measured equivalence ratios were high throughout the experiment, which may be due to calibration of equipment, but equivalent ratios above the upper flammability limit were possible in the Bunsen burner because necessary air can diffuse into the flame from the surroundings once the mixture hits ambient conditions.

**Figure 1: Flame response to varying equivalence ratio**

![Images of flames](image)

At a fuel flow of 80±1 mL/min, liftoff fuel flow reading was determined to be 71±1 mL/min. When the hexagonal flame stabilizer was removed, a liftoff air flow velocity of 68±1 m/s was determined at the same fuel flow rate. The flame stabilizer caused a 4.5% increase in airflow capability.

Flame propagation speed was calculated to be 106 cm/s ±10 cm/s. The length of the tube was estimated, which is a large source of error. Other sources of error included the timing of the video, but was is less than 0.1 second and can be ignored when compared to the error from the estimation of the tube length. Calculated flame...
propagation speed was higher than expected. Deviations from this may have been due to more turbulent nature of our laboratory flame, especially after the flame had traveled to the bottom of the tube and lost some of its purely laminar features. Also, error from tube measurement may have skewed results. Maximum laminar flame propagation speed are typically at an equivalence ratio of 1 and, for propane, are 44 cm/s.

A glass tube allowed for observation of blowback phenomena. When fuel flow was cut off, the flame front was observed propagating downwards.

The effect of a mesh below critical diameter was observed. When the mesh was placed two inches about the flame, flame did not propagate down to the tip of the Bunsen burner because the mesh had a diameter below the critical diameter for propane at conditions in the laboratory.

Conclusion:
The effect of equivalence ratio on flame shape, color, and structure of a propane Bunsen burner flame was examined. Liftoff conditions, blowback and detonation phenomena were observed. Laminar propane flame propagation speed was calculated, and the effect of sub-critical diameter mesh on flame behavior was shown all utilizing a Bunsen burner combustion training apparatus with propane fuel.

Flame structure varied with equivalence ratio. Soot formation caused a bright orange glow when no air flow was present, and blue intensity increased with decreasing equivalence when air was supplied. Detonation and the effect of a sub-critical diameter mesh were also observed. Liftoff air flowrate was determined to be approximately 71 mL/min with the flame stabilizer and 68 mL/s without. The stabilizer provided 4.5% more airflow without blow off. Flame propagation was prevented by the sub-critical diameter mesh. Laminar flame propagation was calculated to be 106 cm/s ±10 cm. Tube length was estimated, so accuracy is limited. Calculated equivalence ratios were unusually high throughout the experiment.

Questions:

1. The flame stabilizer allowed the flame to remain attached at 4.5% higher flow rates in this experiment. In general practice, the function of a flame stabilizer is to decrease local flow velocities via boundary layer formation and to produce recirculation zones that air in the anchoring of flames[1-2]. Flame stabilizers create a geometry that aids in the formation of local turbulent zones where ignition of fresh reactants occurs readily[2]. Furthermore, local recirculation zones cause by this turbulence re-circulate heated products back to the base of the flame before they propagate away from the burner, which raises local temperature and anchors the flame[2].

2. A flame is a zone of finite thickness where rapid chemical reactions occur [1]. As reactant species approach a flame, they are said to be in the pre-heat zone [1]. When species reach the flame front, they are in the reaction zone. The reaction zone is where the majority of heat release, and therefore visible radiation, occurs due to the destruction and recombination of chemical bonds[1][3]. The reaction zone gives a flame its color due to the chemical species being excited in the region [3]. For hydrocarbon flames, such as that of propane, chemistry is dominated by three body recombination reactions and the conversion on carbon monoxide and hydroxide to carbon dioxide and hydrogen by the chemical reaction CO + OH --→ CO₂ + H [1][3].

When there is excess air, the flame appears blue due to excited CH radicals [1][3]. When less air is supplied, the resulting fuel rich flame appears blue-green due to excited C₂ [3]. OH also contributes to the visible spectrum, along with the chemiluminescence from the reaction of carbon monoxide with oxygen radicals [3]. When air is reduced even more, soot forms, which scatters infrared light [3]. The human eye’s sensitivity perceives this radiation as orange-white, which is what was observed for a diffusion flame [1].
3. Balanced equation for the complete combustion of hydrocarbon:

\[ C_xH_y + a(O_2 + 3.76N_2) \rightarrow xCO_2 + (y/2)O + 3.76aN_2 \]

\[ a = x + y/4 \]

Balanced equation for complete combustion of propane:

\[ C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2 \]

Flames will only propagate if the relative amounts of fuel and air present are within the particular fuels flammability limit. Flame will not propagate if equivalence ratio is too high (upper limit) or too low (lower limit) [2]. At the upper limit, the fuel dilutes the oxygen required for combustion to occur [1-2]. Near the lean limit, heat is lost to surrounding air such that temperature cannot reach a level that sustains combustion [1]. Upper (rich) flammability limit for propane is 2.83 and the lower (lean) flammability limit is 0.51 according to [1]. Observed equivalence ratios were much higher than the theoretical upper flammability limit. In most environments, flames can exist above this limit because reactants diffuse into the flame from the surroundings, which sustains combustion.

4. Main differences between flame propagations and detonations include the speed of the propagation, the difference between initial and final pressure, and differences between velocities entering and leaving flame [1]. Detonation velocity is significantly faster than flame propagation speed by a factor of over 6,000 [1]. Pressure of species following flame propagation is nearly the same as before the propagation reaches species, while pressure after a detonation propagates is 13-55 times greater than prior to detonation wave [1]. Detonations are also accompanied by higher temperatures following detonation [1]. The velocity of species entering a detonation wave is greater than the species leaving, while species have a higher velocity than they entered a propagation wave with [1].

5. Soot particles are made up primarily of carbon and are, in simple terms, the result of incomplete combustion [1]. The formation of soot is chemically complex but can be broken down into 4 steps: formation of precursor species, particle inception, surface growth/particle agglomeration, and particle oxidation [1]. Soot precursor species include polycyclic aromatic hydrocarbons, which grow via reactions involving acetylene until the particle inception step is reached [1]. The particle inception step is when the soot molecule reaches a critical size (3,000 – 4,000 atomic mass units) to be considered a particle [1]. Growth occurs both chemically and through coagulation [1]. Particles continue to experience surface growth as they move up through the flame region, which is the third step [1]. In the fourth step, soot particles must cross the oxidation zone, which in a Bunsen burner flame is the flame tip [1]. If all particles are oxidized, the flame does not produce soot, but incomplete oxidation of soot particles is what characterizes a soot-producing (sooting) flame [1].

Soot formation is important in heat transfer of combustion systems because the greatest portion of energy radiated by flames lies in the infra-red portion of the electromagnetic spectrum [3]. Soot particles radiate infrared light with maximum intensity in accordance with Wien’s law due to particle size [1][3]. Because most radiation is in the infrared, soot particles allow for increased radiative heating, which is important in boilers, where the heat released must scatter in many directions in order to transfer to water efficiently [1][3].
References:


