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DIFFUSION FLAME STUDIES OF SOLID FUELS WITH NITROUS OXIDE

A Thesis in

Mechanical Engineering

by

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ABSTRACT

Fundamental counterflow combustion studies and static-fired rocket motor experiments were conducted to investigate baseline solid fuel (hydroxyl-terminated polybutadiene, HTPB) and aluminized solid fuel combustion under varied pressure environments using gaseous oxygen (GOx) and nitrous oxide (N₂O). Combustion experiments were coupled with a detailed model developed to understand GOx and N₂O combustion with pyrolyzing HTPB under pressurized environments.

The pressure influence on N₂O decomposition is studied in detail describing the flame structure, and solid fuel combustion. Counterflow combustion experiments and model results show solid fuel regression rate increases with pressure for a fixed momentum flux. The flame structure thins, due to the faster kinetics, and shifts towards the regressing fuel surface with increasing pressure. Flame temperature increases with pressure as well, due to decreasing radical formation, increasing the surface temperature gradient, resulting in enhancement of solid fuel pyrolysis. Heat release from N₂O decomposition and pyrolyzed fuel oxidation occurs in two distinct stages under atmospheric conditions, while at elevated pressure (1.827 MPa) the exothermic peak associated with oxidation becomes distributed over a wide spatial domain containing many reactions with large exothermicities. The flame structure with N₂O exhibits the same trends as O₂ following decomposition. Leakage of O₂ and NO into the fuel pyrolysis zone also decreases with increasing pressure, indicating faster reaction rates. Over the range of pressures investigated, the diffusion flame produced by combustion of HTPB pyrolysis and N₂O decomposition products was always positioned on the oxidizer side of the stagnation plane, which also shifted toward the fuel surface with increasing pressure.

Aluminized solid fuel combustion experiments coupled with spectroscopic analysis of the flame zone detected AlO emission only when combusted with gaseous oxygen, indicating ignition of the aluminum was not achieved using N₂O, and/or significant amounts of aluminum were not leaving the fuel surface. With both oxidizers, aluminum was observed to collect in the melt layer formed on the solid fuel surface.

Motor combustion experiments were conducted to evaluate the propulsive performance of N₂O/HTPB and N₂O/aluminized HTPB system having a 6.5 and 26 μm Al particle size, with loading up to 10% by weight. Average linear regression rates were observed to increase by 15% over the HTPB baseline for an average N₂O momentum flux of 60 kg/m²s.

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NOMENCLATURE

a	Fuel Specific Regression Rate Coefficient
Al	Aluminum
Al_2O_3	Aluminum Oxide
A^*	Nozzle Throat Area
A_o	Average Initial Cross-Sectional Area of the Gage Section
A_p	Initial Port Area
c^*	Characteristic Velocity
c^*_{ideal}	Ideal Characteristic Velocity
GOx	Gaseous Oxygen
$\overline{GOx}$	Time Averaged Oxidizer Mass Flux
HAN	Hydroxylammonium Nitrate
HPCL	High Pressure Combustion Laboratory
HTPB	Hydroxyl-terminated Polybutadiene
I_{sp}	Specific Impulse
$I_{sp,vac}$	Vacuum Specific Impulse
I.D.	Inner Diameter
LGCP	Long-Grain Center-Perforated Hybrid Rocket Motor
LSHR	Lab Scale Hybrid Rocket Motor
$\overline{\dot{m}}_f$	Time Averaged Fuel Mass Flow Rate
M_i	Initial Fuel Grain Mass
$\overline{\dot{m}}_{ox}$	Time Averaged Oxidizer Mass Flow Rate

MW	Molecular Weight
n	Fuel Specific Regression Rate Power Law Exponent
η_{c^*}	c* Combustion Efficiency
NASA CEA2	NASA Chemical Equilibrium with Applications Version 2
O.D.	Outer Diameter
O/F Ratio	Oxidizer to Fuel Ratio
$\bar{P}_c$	Time Averaged Chamber Pressure
PCBE	Pressurized Counterflow Burner Experiment
PSU	Pennsylvania State University
$\dot{r}$	Regression Rate
$\bar{\dot{r}}$	Time Averaged Regression Rate
r_f	Final Port Radius
r_i	Initial Port Radius
SP	Straight Port
t_b	Burn Duration
T_f	Flame Temperature
wt%	Percentage by Weight

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DEDICATION

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CHAPTER 1: Introduction

1.1 Background

1.1.1 Hybrid Rockets

There are two different types of rocket propulsion systems readily used today: electric and chemical propulsion systems. Chemical propulsion, however, is the predominate system used in launch applications due to the high thrust-to-weight ratio. There are three types of chemical rockets: solid, liquid, and hybrid rockets. A solid rocket contains both the fuel and oxidizer intimately combined in solid form, being either homogenous (molecular mix, such as double base propellant) or heterogeneous (particle/binder matrix, such as composite propellants). A system is considered to be a liquid rocket when both the fuel and oxidizer, stored separately, are in liquid form. A hybrid rocket is a combination of a liquid and solid rocket. Classical hybrid rockets employ an inert solid fuel and liquid or gaseous oxidizer separately stored, with the solid fuel being stored in the combustion chamber [1]. Diagrams of the three types of chemical propulsion rockets including liquid, solid, and hybrids are shown in Figure 1.1.

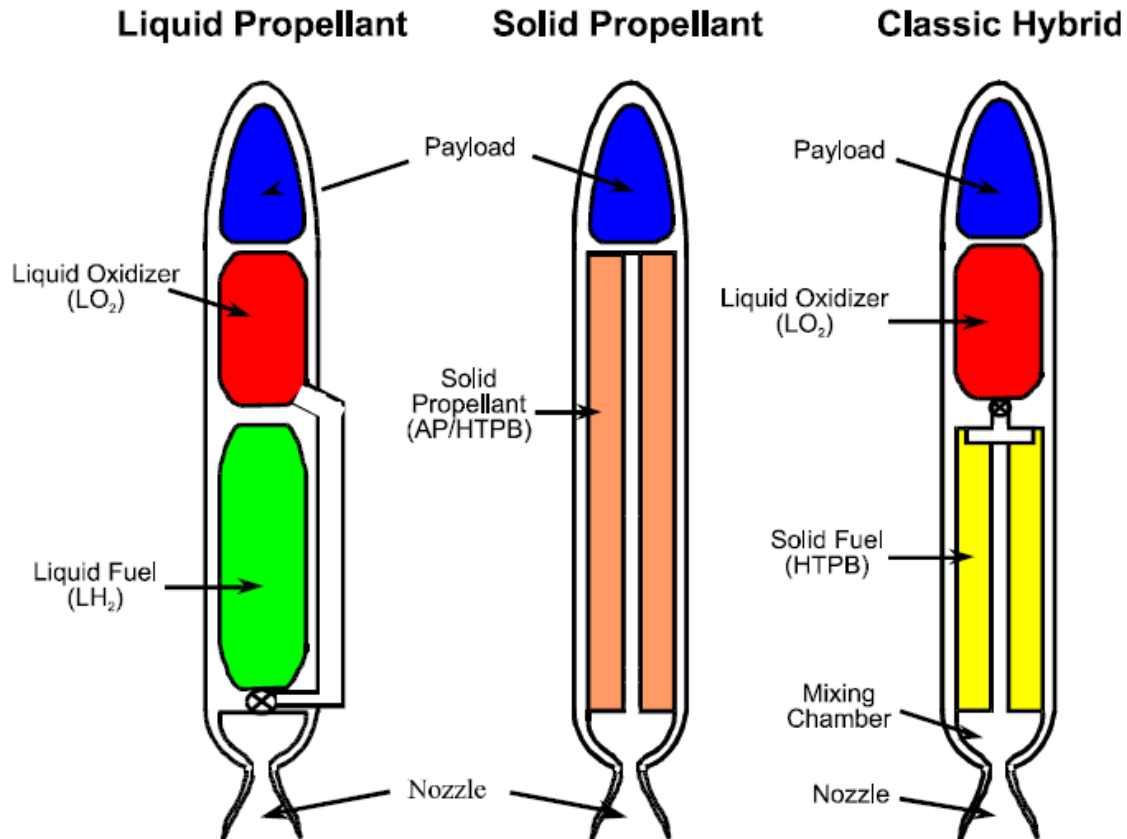


Figure 1.1: Classical hybrid rocket configuration compared to liquid and solid rockets [2].

Hybrid rocket propulsion systems have many advantages over the conventional liquid and solid propellant rockets. One major advantage is the inherent safety over the solid rocket since the fuel and oxidizer are physically separated, and can therefore not react except when the rocket is being fired [3]. This characteristic allows for on-off operational capabilities as well as the ease of being throttled. Thus, the hybrid rocket mission can be aborted non-destructively at any point, whereas a solid rocket, once ignited, will burn until the solid propellant is depleted. Also, unlike liquid propellant rockets, hybrid rockets require less plumbing (only for the oxidizer) resulting in reduced complexity [1].

Overall, hybrid rockets have higher specific impulse compared to solid propellant rockets and higher density-specific impulse compared to liquid rockets [1] [3]. One of the main disadvantages of hybrid propulsion is the low regression rates associated with the solid fuel combustion causing relatively low thrust values (i.e, a large burn-surface area is required to achieve a given level of thrust) [3]. The low mass regression rates are due to the low densities of the fuels, and the diffusion-controlled combustion process. Once ignited, the pyrolyzed fuel mixes and combusts with the oxidizer that is injected and forms a diffusion flame depicted in Figure 1.2. Not only do hybrids suffer from low regression rates but the O/F ratio changes during a motor firing due to the increasing fuel surface area with time [4]. Hybrid rocket propulsion system development is premature compared to that of liquid and solid propulsion systems resulting in a lack of understanding of combustion behavior in hybrid rocket motors [5] .

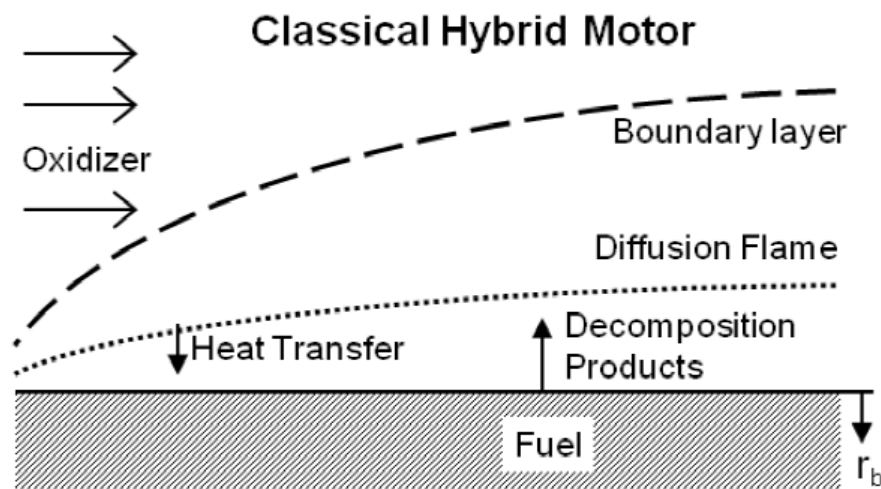


Figure 1.2: Classical hybrid combustion schematic [6].

To enhance the performance of hybrid rockets, several techniques have been investigated including: addition of energetic particles into the solid-fuel grain; replacement of the inert hydroxyl-terminated polybutadiene (HTPB) binder with energetic polymers [e.g., glycidyl azide

polymer (GAP)]; and the substitution of the oxidizer with a more dense liquid oxidizer such as hydroxyl ammonium nitrate (HAN) [4]. Although replacing an inert binder with an energetic polymer may increase the overall performance, it will diminish the overall safety of the hybrid rocket system. Therefore, a desirable way to improve the performance of a hybrid rocket is to employ energetic particles in the inert solid fuel to increase the energy density.

1.1.2 Metal Particle Combustion

Metal particle addition to the solid fuel can enhance the performance of hybrid propulsion systems by providing a high heat of combustion (a desirable combustion property) as well as a high fuel density. High density is desirable since it increases performance for the same volumetric capacity [7]. Rockets are volume-limited systems; therefore the more energy input for the same amount of volume is desirable. Metal particles also increase the flame temperature which may, as shown in Eq. 1.1, increase specific impulse, I_{sp} . Even though metal particles can increase the flame temperature (T_f), the increase in molecular weight (MW) of the products with the addition of metal particles may diminish the effect of a higher I_{sp} . Metal particles, however, have the potential to improve performance for many hybrid systems, as well as dampen internal pressure oscillations due to the drag created by the condensed-phase products [8].

$$I_{sp} \propto \sqrt{\frac{T_f}{MW}} \quad (1.1)$$

Although the I_{sp} may not increase significantly with metal particles, the density I_{sp} will have a significant increase. The density I_{sp} is provided in Eq. 1.2.

$$I_{sp,density} = \rho I_{sp} \quad (1.2)$$

where ρ is the aggregate density of the fuel and oxidizer.

Many metal particles have been considered by researchers for applications in propellants (aluminum, boron, magnesium, etc.). The heat of oxidation of several common fuels, both gravimetrically and volumetrically, are given in Figure 1.3.

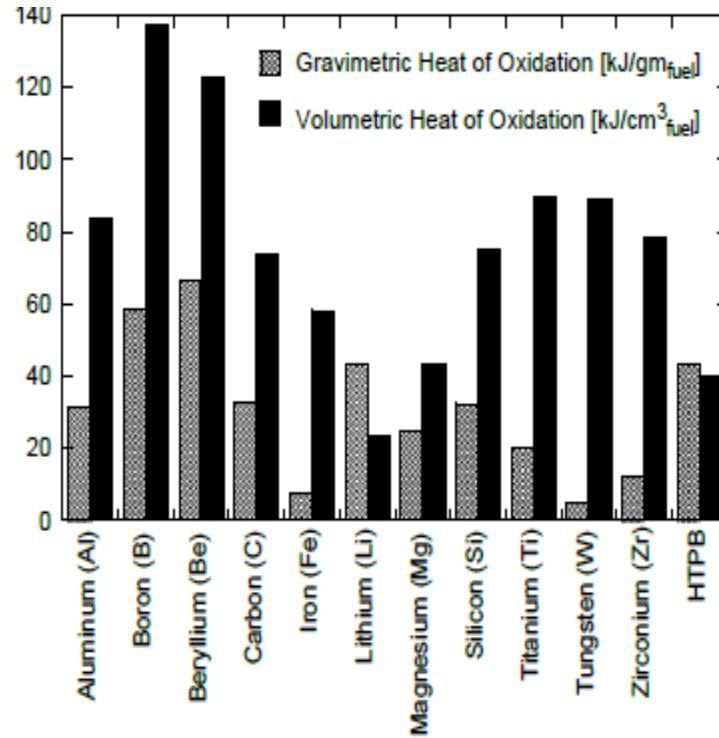


Figure 1.3: Comparison of heats of combustion with oxygen of several fuels [4].

Boron initially seems to be the best viable option having the highest volumetric heat of oxidation, however; there have been difficulties with ignition, and complete conversion to liquid boron oxide. The subsequent candidate, beryllium, generates a highly toxic byproduct, beryllium oxide. Therefore, aluminum is the best viable option [8].

The greater energy release from the oxidation of the metal particles shows a substantial increase in regression rate compared to non-metalized solid fuels. However, like all metals, an oxide layer on the outer particle surface serves to passivate the pure metal under ambient conditions, and must be removed before full combustion with the metal can occur at an

appreciable rate. Removal of this thin layer, either by melting or vaporization, increases the ignition time delay. As the particle size is reduced, the thickness of the passivating oxide layer remains nearly constant resulting in an increase of the oxide weight percentage to over 50% for nanoscale additives (~50 nm diameter). Furthermore, as the particles become smaller, the wetted surface area increases for a given particle mass loading and thus the fuel mixture viscosity increases making solid fuel processing more difficult. These are some of the drawbacks of having particle additives, which will be discussed later.

1.1.3 Aluminum Combustion

To understand why regression rate increases with metal particle addition, the combustion behavior of aluminum must be understood. Aluminum particles have an aluminum oxide (Al_2O_3) shell passivating the solid aluminum core. Once this oxide layer is ruptured or cracked, exposing the aluminum to the oxidizing atmosphere, rapid oxidation, ignition, and combustion occur. This rupture can be caused by two different events. The aluminum oxide melting temperature of 2327 K is much higher than the melting of aluminum at 930 K. Therefore, the aluminum oxide must reach high enough temperature to melt on its own. Otherwise, stresses created from the expansion of aluminum upon melting inside the oxide shell could fracture the oxide shell, exposing the pure aluminum to surrounding oxidizer and allowing ignition [9]. The various stages of aluminum particle ignition are shown in Figure 1.4.

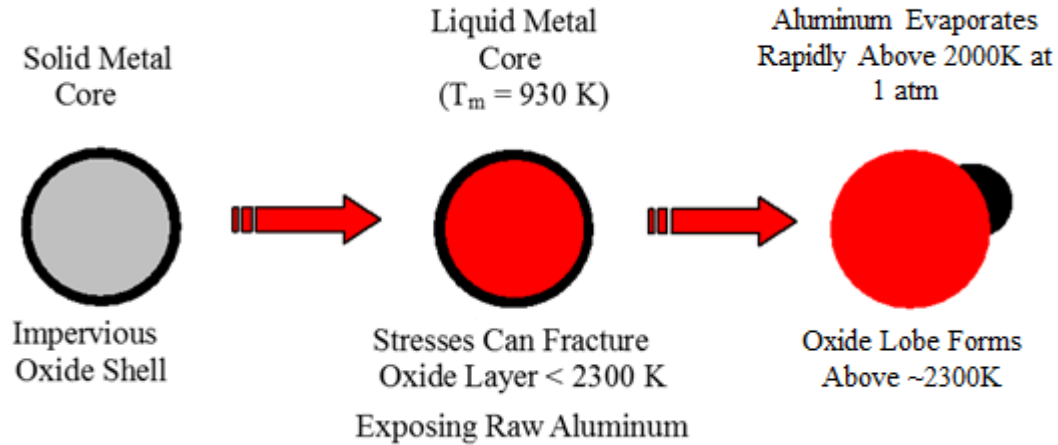


Figure 1.4: Traditional aluminum ignition and combustion [10].

As the aluminum is heated, the aluminum inside the solid metal core starts to deform and liquefy, becoming egg-like, with the oxide shell preventing the molten aluminum from reacting with the environment. The lower density of the molten aluminum stresses the oxide shell forcing the shell to fracture, exposing the liquid aluminum core.

As the temperature exceeds the oxide melting temperature, tension draws the oxide into a lobe on the droplet surface, allowing the now exposed aluminum to react with the surrounding environment. The heat release from surface oxidation continues to raise the particle temperature to temperatures close to the aluminum boiling point temperature, thus enabling vigorous vaporization. Dreizin determines aluminum ignition may initiate due to phase transition of Al_2O_3 , producing a higher density oxide phase which forms cracks, allowing oxidizer to diffuse into and react with the neat particle core [11].

With nano technology on the rise, researchers are interested in investigating nanoparticle additives. These nanoparticles have some advantages over micron-sized additives. The smaller the particle, the faster it reaches the vaporization temperature. Other advantages include:

- 1) Shortened burning times
- 2) Higher surface area enhancing heat transfer and reaction rate
- 3) Reduced ignition delay

Enhancement of solid fuel regression rate due to metallic particle additives was experimentally investigated by Risha at the High Pressure Combustion Lab (HPCL) using the Long Grain Center Perforated Hybrid Rocket Motor (LGCP). The test matrix contained a total of 19 different aluminized HTPB fuels. Out of all the formulations, the two that showed the largest increase in regression rate were HTPB containing 13% micrometer-sized Al particles and 13% Alex[®], a nanosize aluminum particle made by the exploding wire process [12]. The Alex[®] containing fuel demonstrated an increase of 123% in linear regression rate over the baseline HTPB [8]. The addition of aluminum also increases the mass regression rate, where the addition of 20% Alex[®] powder to HTPB solid fuel increased the mass burning rate by 70% [4]. From such studies, the enhancement in solid fuel regression rate due to the introduction of aluminum particles, as well as particle size effects, is evident.

Despite the overall benefits of nanoparticle additives they also possess undesirable characteristics. As mentioned previously, all metals have an inert oxide layer encasing the neat metal core. The weight percent (wt%) of this oxide layer increases as particle diameter is reduced. With such a high surface area to volume ratio, this can significantly increase the viscosity of the fuels making processing fairly difficult. Therefore, when considering metal particle addition to a solid fuel grain, the size of the particle becomes an important decision in

the process. Along with deciding the metal particle sizing, the actual fuel and oxidizer become important parameters to focus on when designing a hybrid rocket motor.

1.2 Nitrous Oxide as an Oxidizer

Hybrid rocket motors can be used for a variety of different mission scenarios. With the chosen mission scenario comes determining the correct fuel and oxidizer combination. For example, liquid oxygen (LOx) oxidizer and HTPB fuel are used for large hybrid booster applications; while HTPB and hydrogen peroxide are used for lower energy upper stage rockets [13].

Two of the most popular oxidizers currently in use today for hybrid propulsive systems are LOx and nitrous oxide (N_2O), due to their safety (low toxicity), cost, and availability. N_2O has become a new-found favorite oxidizer used in hybrid rocket motors due to its self-pressurizing capability [14].

N_2O , when stored at room temperature ($20^\circ C$), has a vapor pressure of approximately 5 MPa (730psia). With such a high vapor pressure, the self-pressurizing N_2O eliminates the need for helium as a pressurant. Therefore, N_2O is normally used in small rocket systems. LOx has the advantage of yielding a high specific impulse compared to N_2O .

The disadvantage of LOx is the cryogenic storage temperature requirement, of a temperature below 90.15 K, whereas N_2O has reduced I_{sp} performance, compared to LOx since 2/3 of N_2O is nitrogen, which is an inert gas. N_2O can also become a hazard due to its exothermic decomposition reaction [15] [16]. This exothermic behavior creates benefits in terms of the motor stability and efficiency characteristics, but can present an explosion hazard [17].

1.3 Research Goals

N_2O is currently being considered for use in a wide range of sounding rockets for hybrid rocket motor applications. Considerably less fundamental research is available on N_2O as an oxidizer in hybrid motors. Of particular interest is the behavior of N_2O as a function of pressure and the resulting effect on the diffusion flame structure with solid fuels such as HTPB.

Furthermore, the addition of metal particles embedded in the solid fuels using N_2O as the oxidizer has had even less study. For example, it is still not known if metal additives will accelerate the burning of the solid fuel, as had previously been demonstrated with pure oxygen. To improve the overall performance for future (small scale) motors, a better understanding of the combustion process with N_2O as an oxidizer is required. The goal of the present research is to understand the diffusion flame behavior of N_2O , with HTPB fuel along with the addition of aluminum particles, utilizing counterflow burners, hybrid rocket motors, and numerical modeling. The specific tasks for this project included:

- Perform experiments in a counterflow burner under atmospheric conditions with HTPB and aluminized HTPB using N_2O to determine whether there is an improvement in linear regression rate.
- Perform experiments in a pressurized counterflow burner to evaluate pressure effects on regression rates, applicable to that of a hybrid rocket motor.
- Perform static-fired hybrid rocket motor experiments with N_2O as the oxidizer, using both HTPB and aluminized HTPB fuels.
- Perform modeling studies of the counterflow burner for pure HTPB to understand the N_2O flame structure at relevant experimental conditions and compare these results to those with O_2 as the oxidizer.

CHAPTER 2: Background and Motivation

2.1 Combustion Process for a Hybrid Rocket Motor and Counterflow Burner

As mentioned previously and as shown in Figure 1.2, the combustion process of a hybrid fuel grain is fundamentally a diffusion flame problem with crossflow. The hybrid rocket is complex due to the interactions between physical phenomena. The interactions include solid fuel pyrolysis, gas phase diffusion, mixing and combustion, heat transfer through convection, conduction, and radiation, as well as turbulent and laminar flow with varying flow channel configuration.

In a hybrid rocket, the oxidizer is sprayed or injected into the fuel grain port where a thin flame sheet forms inside of the gaseous flow boundary layer, with the flame height above the surface located around 10 to 20% of the boundary layer thickness. The flame sits close to stoichiometric conditions and is fed from below by the vaporization/decomposition of the fuel and above from the convective flow of the oxidizer. The two important factors to take into consideration are the flame location in the boundary layer and the heat of gasification, since the regression rate is controlled by heat transfer from the flame to the fuel. The regression rate is proportional to this heat transfer to the wall:

$$\rho_f \dot{r} = \dot{Q}_w / \Delta H \quad (2.1)$$

where ρ_f is the density of the fuel, $\dot{r}$ is the linear regression rate, $\dot{Q}_w$ is heat transfer per unit area to the wall and ΔH is the effective heat of gasification of the solid fuel. The fuel is continuously being gasified from the heat generated by the diffusion flame, by both convective and conductive heat transfer. Fuel vaporization resulting from the heat flux is independent of any transport mechanism and reaction rate when the Lewis number (Le) is one, when the boundary layer is laminar, and turbulent. Therefore, the regression of the fuel is through conduction:

$$\dot{Q} = -k \frac{dT}{dy} \quad (2.2)$$

where $\dot{Q}$ is the heat flux per unit area, k is the thermal conductivity of the fuel, and y is the direction normal to the fuel surface into the gas phase. This equation holds true for either turbulent or laminar flow, k being changed for the appropriate flow. The constant vaporization of the fuel surface at a relatively high velocity creates a so-called “blowing” effect, which limits the burning rate, reducing the heat transfer to the surface. This modification in heat transfer to the surface can be appropriately defined by a Stanton number ratio. The Stanton number, C_H , is a measure of heat transferred into a fluid relative to the thermal capacity of that fluid. The Stanton number ratio (C_H/C_{Ho}) is the Stanton number ($h/\rho V c_p$) divided by the Stanton number without the blowing effect, C_{Ho} . The Stanton number is defined in terms of the mass flux and enthalpy at the flame, which leads to a separate parameter, u_e/u_c , which relates the regression rate to the flame position. Therefore, the wall heat flux in terms of the Stanton number ratio is defined by:

$$\dot{Q}_w = C_{Ho} \frac{C_H}{C_{Ho}} \rho_c u_c (h_{c,s} - h_{w,g}) \quad (2.3)$$

where $\rho_c u_c$ is the axial mass flux at the combustion layer, $h_{c,s}$ is the stagnation enthalpy at the flame, and $h_{w,g}$ is the enthalpy at the wall in gas phase. The Stanton number ratio, $\frac{C_H}{C_{Ho}}$ accounts for the reduction in heat transfer due to blowing. The blowing effect also causes the critical Reynolds number for transition to turbulent flow to decrease, making the flow in the hybrid motor boundary layer turbulent over most of the fuel grain length [18].

A relation can be made between the Stanton number and the friction coefficient consistent with hybrid combustion, where the Stanton number becomes:

$$C_H = \frac{1}{2} C_f \left(\frac{\rho_e u_e^2}{\rho_c u_c^2} \right) \quad (2.4)$$

where C_f is the local skin coefficient. The friction coefficient is approximately the same as that with an ordinary boundary layer with or without blowing therefore C_{Ho} becomes:

$$C_{Ho} = C Re_x^{-0.2} \left(\frac{\rho_e}{\rho_c} \right) \left(\frac{u_e}{u_c} \right)^2 \quad (2.5)$$

where $C \approx 0.03$ and Re_x is the Reynolds number, $\left(\frac{\rho_e u_e x}{\mu} \right)$. Equations 2.2 and 2.5 describe the heat transfer from the flame to the fuel surface; according to Eq. 2.1, the regression rate can then be expressed as:

$$\dot{r} = \frac{C G Re_x^{-0.2}}{\rho_f} \left(\frac{C_H}{C_{Ho}} \right) \frac{u_e}{u_c} \frac{(h_{c,s} - h_{w,g})}{\Delta H} \quad (2.6)$$

with the primary mechanism being heat transfer to the fuel surface from the diffusion flame, the classical hybrid motor fuel regression rate analysis by Marxman is given by:

$$\dot{r} = \frac{1}{\rho_f} \frac{C_f}{2} G B \quad (2.7)$$

where C_f is the blowing friction coefficient, G is the mass flux, and B is the blowing coefficient [19].

Therefore, the actual combustion process of a hybrid motor can be itemized to describe the overall process with many of the processes occurring simultaneously:

- Thermal heating and pyrolysis of the solid fuel
- Decomposition and breakdown of the fuel
- Diffusion of fuel species to the flame zone, creating a diffusion flame
- Formation of boundary layer due to turbulent mixing near solid fuel grain
- Diffusion of oxidizer to fuel surface creating heterogeneous reactions
- Fuel grain continuing to regress due to heating from the turbulent diffusion flame
- Changing surface area and mass flux of fuel due to fuel regressing

- If metal particles are in the fuel, potential ejection of unburnt residue [20]

The list shows many of the physical and chemical processes of combustion in a hybrid rocket motor. That being said, the reaction of the gas is often considered, theoretically, to occur infinitely fast causing the Damkohler number (a ratio of the fluid dynamic time scale to chemical reaction time scale) to be much greater than one implying that combustion is diffusion-controlled. However, when metal particles are added to the solid fuel, the combustion time of the particles takes longer, decreasing the Damkohler number, potentially requiring a post-combustion chamber to be inserted downstream of the fuel grain to increase the residence time available to fully burn the particles within the chamber.

Although a hybrid rocket motor exhibits a counterflow flame in cross flow, it is different than a pure counterflow flame. Counterflow combustion experiments have been used in numerous studies of non-premixed flames to determine extinction limits with its one-dimensional diffusion flame structure. It is a flame where a uniform oxidizer jet impinges against a uniform fuel jet [21]; or in the case of this study, a solid fuel that is vaporizing and decomposing as shown in Figure 2.1.

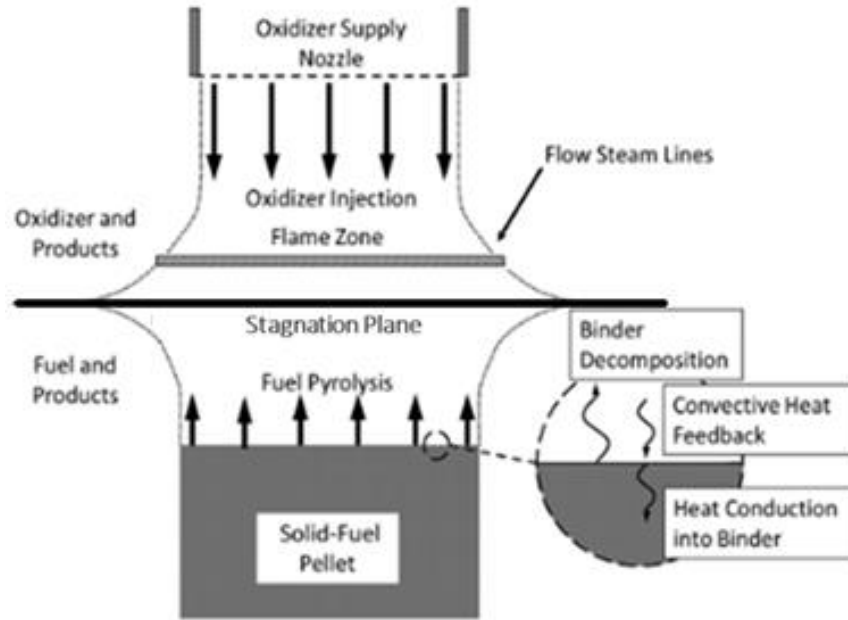


Figure 2.1: Diagram of opposed-flow non-premixed flame [19].

The stagnation surface, also known as the stagnation plane, is located between the fuel and oxidizer, where the two velocities go to zero. The oxidizer and fuel density and velocity are usually different, causing the stagnation line to shift in the appropriate direction. The diffusion flame is located near the stoichiometric mixture fraction. For example, the stoichiometric mixture fraction of an H_2 -air flame being 0.028, positions the flame on the oxidizer side of the stagnation plane due to a lower mixture fraction. The mixture fraction is defined as the total amount of mass stuff from the fuel stream divided by the total mass of stuff, with the mixture fraction in terms of mass fraction of fuel and products given by Eq. 2.8, where Y_f is the mass fraction of the fuel and Y_{pr} is the mass fraction of the products.

$$f = Y_f + \left(\frac{1}{1 + \frac{A}{F}} \right) Y_{pr} \quad (2.8)$$

The mixture fraction can then be re-arranged to be put in terms of the stoichiometric air-fuel ratio, shown in Eq. 2.9.

$$f_{stoich} = \frac{1}{\frac{A}{F_{stoich}} + 1} \quad (2.9)$$

The flame sits near the stoichiometric mixture fraction because it is where the flame temperature is the highest and consequently the reaction rate is the highest. In a purely gaseous system, the fuel and oxidizer are transported to the flame location via diffusion and not convection or buoyancy forces [22]. However, convection forces play an important role when utilizing solid fuels instead of gaseous fuels since it is the convective and conductive heat transfer that degrades the fuel to gas.

The structure of a non-premixed flame consists of three zones, with a reaction zone separating a fuel-rich zone and an oxidizer-rich zone. Figure 2.2 shows a typical configuration for a counterflow opposed flow flame.

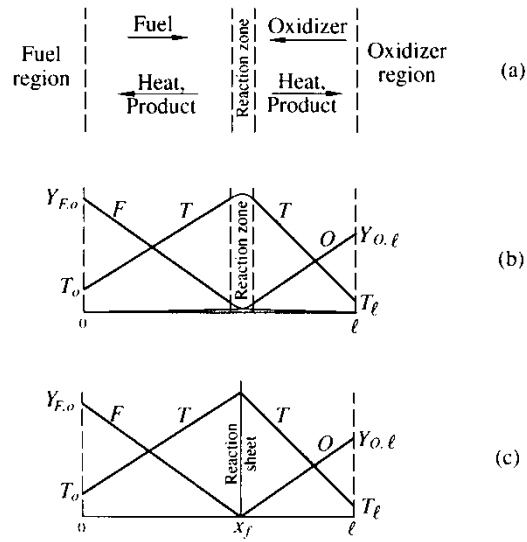


Figure 2.2: Structure of a non-premixed flame: (a) physical configuration of a one-dimensional, purely diffusive system; (b) temperature and concentration profiles with finite flame thickness and reactant leakage; (c) temperature and concentration profiles with reaction-sheet assumption [23].

As the fuel and oxidizer move towards each other by diffusion, they become heated and eventually meet and mix within the reaction zone. The reaction takes place rapidly, and the combustion products are then transported away from the reaction zone in both directions. Since the reaction occurs at a finite rate and the thickness of the flame is finite, a complete reaction does not occur, leaving small amounts of oxidizer and fuel, which leak through the reaction zones as seen in Figure 2.2(b).

If the diffusion and convection times are less than reaction times, the reaction may be assumed to occur infinitely fast which confines it to a reaction sheet as shown in Figure 2.2(c). The fuel and oxidizer are confined to their respective regions of supply and vanish at the reaction sheet, where no leakage occurs. The reaction sheet then acts as a sink for the reactants and a source of combustion heat and products [23].

An important parameter associated with counterflow flames is the strain rate as defined in Eq. 2.10.

$$Ko = \frac{(u_o)}{L} [1 + (\frac{u_f}{u_o})(\frac{\rho_f}{\rho_o})^{1/2}] \quad (2.10)$$

This equation applies when the flame is on the oxygen side of the stagnation plane, which in the current study is where the flame forms, given the stoichiometric mixture fraction, which will be discussed in section 6.2. In the equation above the strain rate, K , is in units of inverse time, ρ is the density, u represents the velocity at the exit plane of each reactant, the subscripts o and f refer to the oxidizer and fuel, respectively, and L is the separation distance between the fuel and oxidizer exit planes. With increasing strain rate, the flame becomes thinner decreasing the flame temperature and eventually reaching a state of extinction [21]. The strain rate is not as dominant when used in correlation with hybrid rocket motors; however, it plays an important factor when conducting counterflow combustion experiments.

CHAPTER 3: Experimental Method of Approach

3.1 Solid Fuel Formulations and Test Sample Preparation

A total of seven solid fuels were formulated using HTPB binder with up to 30 wt% of aluminum particles added for combustion experiments in two counterflow burners and two hybrid rocket motors. Table 3.1 provides a summary of the fuels evaluated using the counterflow burners, and Table 3.2 displays the fuel grain composition, manufactured for hybrid motor experiments.

The solid fuels that were made for the two counterflow burners were made from a percentage of aluminum consisting of three different particle size distributions: Valimet H2 (6.58 μ m average) and H12 (26.34 μ m average) and Novacentrix nanoaluminum (70nm average). Fifty-gram batches of the HTPB were produced, comprising 90% R-45M and 9% isophorone diisocyanate (IPDI) with 1% triphenyl bismuth (TPB) as a curing catalyst. The batches were hand mixed and vacuum degassed to remove air entrapped during mixing. The mixture was then cured under an elevated temperature environment for two days prior to use.

The fuel grains were manufactured separately and cast into phenolic tubing; Table 3.2 displays the test matrix for the fuel grains that were used for hybrid motor experiments. The mixes, 650 g in weight, produced up to five fuel grains having a particle loading ranging from 0 to 10%. Large fuel batches were mixed using a vertical mixer for approximately fifteen minutes. The viscous mixture was then separated and vacuum degassed for ten minutes to remove air entrapped from mixing, after which the fuel grains were allowed to cure at elevated temperature for two to three days before use. An example of one cured aluminum fuel grain is provided in Figure 3.1. The dimensions of the fuel grain were 152.4 mm in length with a 9.5 mm port diameter, obtained through use of a mandrel.

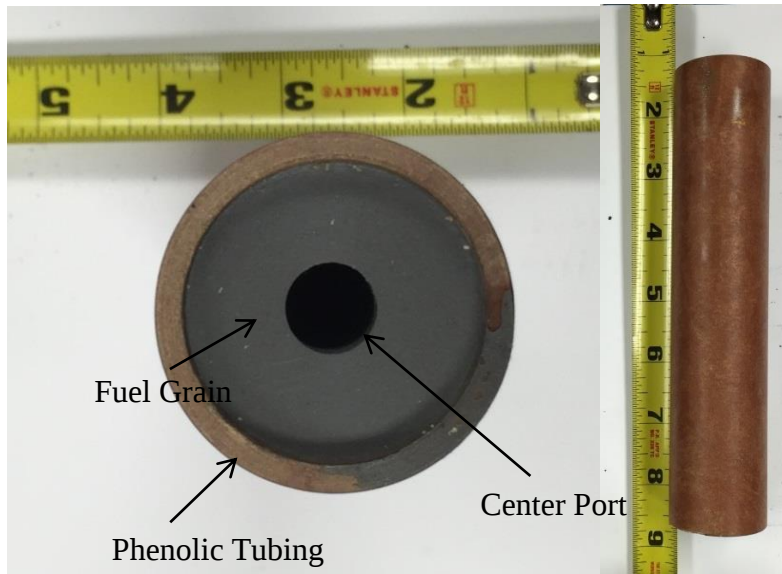


Figure 3.1: Image of one pour-cast HTPB solid fuel grain containing an aluminum loading of 10% H12 used for the current study. The grain has an OD 31.75 mm of (1.25 in) defined by the phenolic casing and a center-port diameter of 9.5 mm (0.375 in) obtained using a mandrel.

Table 3.1: Table of solid fuel pellet composition, manufactured for counterflow burner analysis.

Fuel Designation	HTPB wt%	Additive wt%
SF1	100	N/A
SF2	95	5% H2 Al
SF3	95	5% H12 Al
SF2	90	10% H2 Al
SF3	90	10% H12 Al
SF4	90	10% nano Al
SF5	80	20% H2 Al
SF6	80	20% H12 Al
SF7	70	30% H2 Al

Table 3.2: Table of solid fuel grain composition, manufactured for the hybrid rocket motor experiments.

Fuel Designation	HTPB wt%	Additive wt%
FG1	100	N/A
FG2	90	10% H2 Al
FG3	90	10% H12 Al
FG4	90	10% nano Al

3.2 Experimental Setup

Counterflow burner and static-fired rocket motor experiments were conducted to characterize solid fuel burning rates using GOx and N₂O. Two counterflow burner configurations were utilized, permitting spectral analysis of the flame zone at ambient pressure, as well as combustion under elevated pressure environments. Motor experiments were conducted to characterize propulsive performance of HTPB based solid fuel, having an aluminum particle loading range from 0 to 30 wt%. Two static-fired motors were used depending on firing location (i.e. Naval Surface Warfare Center, Indian Head Explosive Ordnance Disposal Technology Division (Indian Head NSWC), and the HPCL at Pennsylvania State University (PSU)). In the following chapter, each system is described in detail.

3.2.1 Counterflow Burners

Counterflow burner combustion experiments conducted at Indian Head NSWC and PSU were used as a screening method for determining the regression rates of various solid fuel compositions under GOx and N_2O flows. Such experiments were used to simulate the hybrid motor environment with a one-dimensional analysis, as depicted in Figure 2.1. The counterflow burners used in the current study has solid fuel with gaseous oxidizer flowed from opposing, axially aligned, tubes, to observe and characterize the flame structure occurring near the stagnation plane. The counterflow systems often employ a co-flow of inert gas surrounding the fuel and oxidizer to quench the flame and prevent shear-induced mixing, although the counterflow burner at Indian Head NSWC did not have co-flow capabilities. Variation of oxidizer velocity causes the resulting diffusion flame to shift farther or closer to the solid fuel surface, changing the surface temperature gradient and resulting in an enhanced or reduced rate of solid fuel pyrolysis. Flame strain rates may then be varied by altering the oxidizer velocity or the separation distance between the oxidizer flow tube exit and solid fuel surface. A counterflow burner experiment is not an exact one-to-one comparison to a hybrid rocket motor because of the different operating conditions than what is found in a rocket motor, but it allows for the study of fundamental combustion behavior of solid fuels [24]. The counterflow burner configuration allows observation and characterization of the diffusion flame structure occurring near the stagnation plane [25]. A schematic diagram of the counterflow burner without co-flow capability is provided in Figure 3.2.

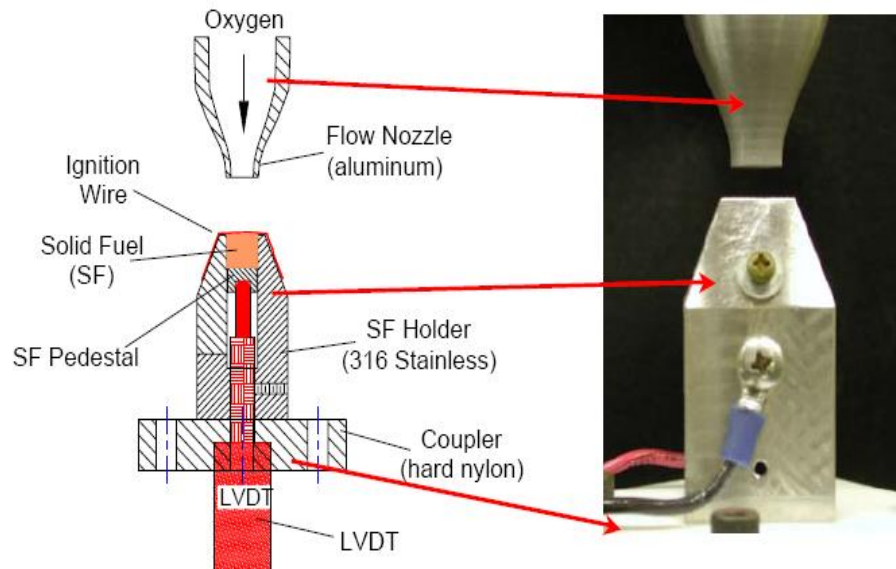


Figure 3.2: Schematic diagram of the counterflow burner without co-flow capabilities [26].

The solid fuel sample was placed onto a pedestal on top of a linear guide, which was in direct contact with a linear variable displacement transducer (LVDT). An axially aligned oxidizer tube was set 5 mm away from the solid fuel surface where the gaseous oxidizer (GOx or gaseous N_2O) flowed. During combustion, the surface of the regressing solid fuel pellet is fixed at the specified separation distance (formation of a surface melt layer can result in a slight reduction of separation distance) by a fine-wire placed across the pellet surface, and by using the compression force of the LVDT spring to keep the surface location constant and track the instantaneous regression rate.

Data was recorded at 1000 Hz using a data acquisition system which tracked the output voltage of the LVDT, which had been calibrated to correlate output voltage to distance. The data was then input into a custom MATLAB program to determine the regression rate. Not only was the axial location of the solid fuel sample monitored, but also a high-precision flow controller was used to set the oxidizer flow rate. An Ocean Optics USB 4000 spectrometer was used to analyze the emission spectra from the flame during the counterflow experiments to determine the

difference in the combustion behavior between the two oxidizers. The spectrometer covered a wavelength range of ~198 nm to 532 nm. Light emission was collected using a one-inch diameter collection lens focused directly on the flame zone.

The pressurized counterflow burner (PCBE) was used to examine the effect higher pressures have on the decomposition and regression rates of HTPB fuels with and without metal additives using N₂O and GOx oxidizers. The PCBE utilized an LVDT to measure the regression of the solid fuel, with a nichrome wire to hold the fuel in place. The separation distance between the fuel surface and oxidizer exit was held constant at 5 mm, although following ignition a thin melt layer formed on the fuel pellet surface causing a slight reduction in separation distance. This reduction in separation distance increases the strain rate as shown in the equation below, thus the ignition and subsequent combustion process is recorded and the actual separation distance is determined for each run by post-processing video analysis. Strain rate was calculated using the following equation [27]:

$$K = \frac{2(u_o)}{L} \left[1 + \left(\frac{u_f}{u_o} \right) \left(\frac{\rho_f}{\rho_o} \right)^{1/2} \right] \quad (3.1)$$

this equation relates the strain rate to the oxidizer side of the flow field since the flame sits on the oxidizer side of the stagnation plane, which will be discussed in section 6.2. The above equation differs from the other strain rate equation, displayed in section 2.1, by a factor of 2 due to the plug flow conditions which correlates more closely to experiments [27]. Figure 3.3 and Figure 3.4 show a block diagram of the PCBE and photographs of the pellet holder base for the PCBE, respectively.

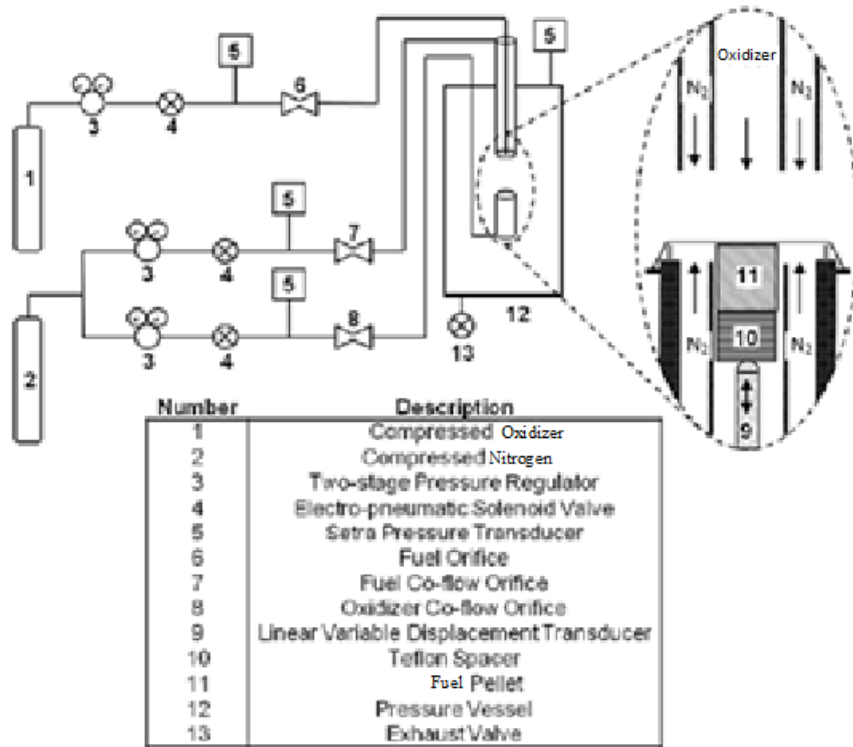


Figure 3.3: Block diagram of pressurized counterflow burner used in this current study [6].

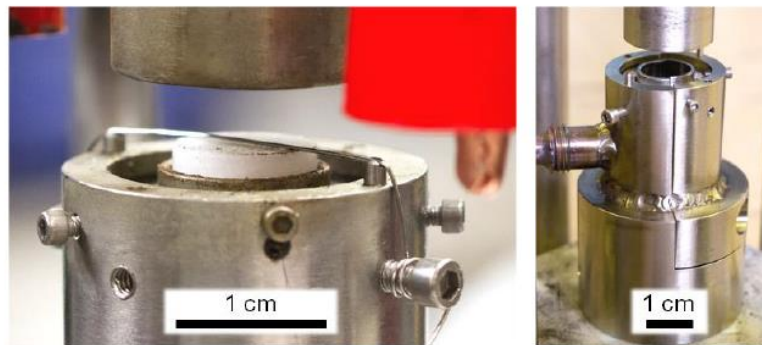


Figure 3.4: Images of pellet holder base for pressurized counterflow burner [6].

Electro-pneumatic solenoid valves and choked flow orifices controlled the flows. To achieve the desired flow rate, required for a given experiment, the pressure upstream of each flow valve was set using remote operated motorized pressure regulators. These pressures were calculated based on a target oxidizer exit velocity, for a specific orifice size and discharge

coefficient, gas type, and exit area. Each orifice was chosen to obtain choked flow, and the co-flows were set to match half of the velocity of the fuel and oxidizer. Calibrated Setra 206 pressure transducers were placed upstream of each orifice as well as connected to porting in the chamber wall to permit determination of gas flow rates into the chamber using choked flow relations with the individual orifice discharge coefficient calibrations, as well as the chamber pressure. The pressure transducer and LVDT signals were recorded using a data acquisition system having a sampling rate of 500 Hz. Figure 3.5 displays an example of a recorded LVDT signal trace obtained from one PCBE experiment. The solenoid valves and ignitor were controlled using a custom LabVIEW control sequencing program to initiate and shut off the flow of gases before and after conducting each experiment.

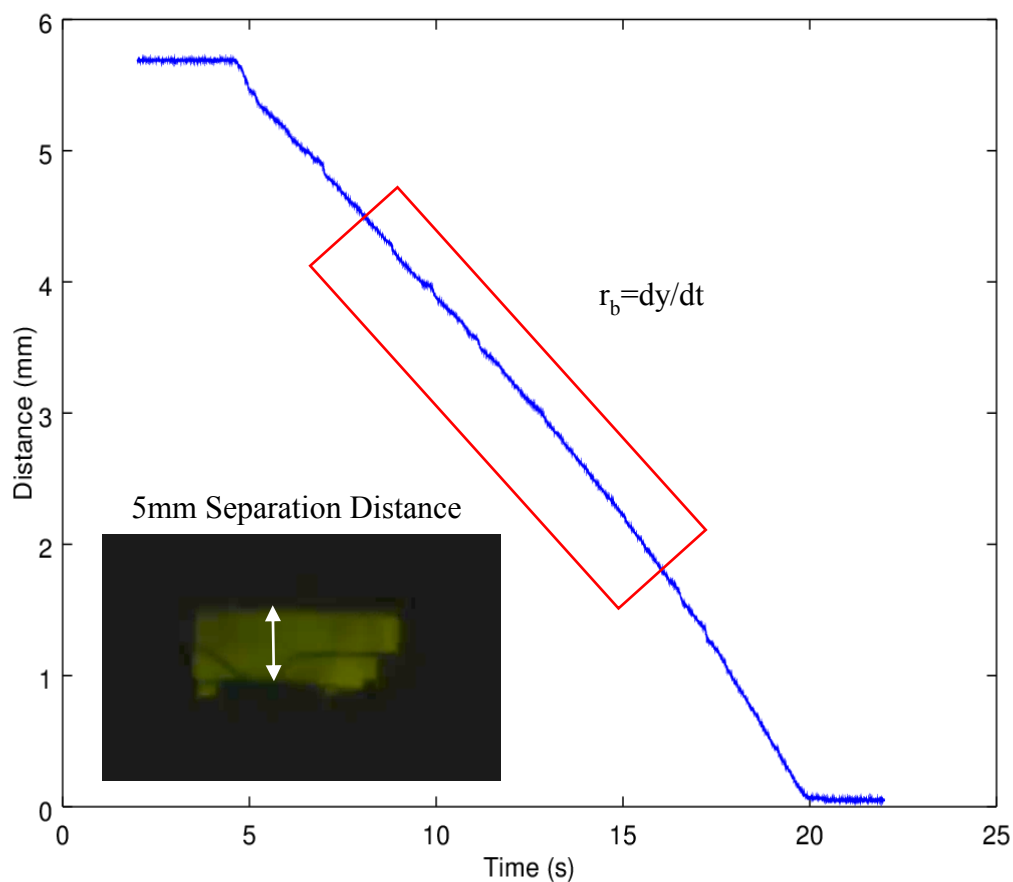


Figure 3.5: LVDT trace obtained from one GOx and HTPB PCBE experiment.

The pellet was held down using a thin nichrome wire which could also be resistively heated to ignite the sample. However, to minimize the possibility of the hold-down wire breaking, a separate nichrome wire was introduced and resistively heated to achieve ignition. Before conducting an experiment, the chamber was purged with nitrogen to remove any entrapped air in the chamber. Once this was accomplished, the chamber was pressurized with nitrogen and allowed to equilibrate at the desired chamber pressure with the oxidizer flow initiated. The nichrome wire was then resistively heated by applying between 8 and 10 vdc across the ignition terminals. By metering the flow through the chamber, the pressure during the

run is held nearly constant. The separation distance and flame structure were recorded using a standard digital video camera located at one of the windows in the pressure vessel.

Post video analysis of the ignition and combustion process indicated the separation distance typically decreased from the initial 5 mm to 3.5 to 4.5 mm once the melt layer formed on the fuel pellet surface. The regression rate of the pellet was determined using the slope of the LVDT profile during the steady state portion of the burn as indicated in Figure 3.5. Using the calculated oxidizer exit velocity and measured regression rate of the fuel, the effect of oxidizer type and pressure may be investigated.

3.2.2 Hybrid Rocket Motors

A Lab Scale Hybrid Rocket (LSHR), designed and constructed at Indian Head NSWC, was employed for conducting fast, accurate motor experiments repeatability in a small-scale package. The main advantage of the LSHR is the ability to investigate various fuels and oxidizers in a modular system which permits a wide experimental matrix to be evaluated with short setup time, allowing multiple firings to be conducted in a short period of time. The LSHR consists of a stainless steel chamber that is 33 cm (13in) long with an 88.9 mm (3.5 in) outer diameter (OD) and 38.1 mm (1.5 in) inner diameter (ID). The internal volume of the combustion chamber is comprised of a pre and post-combustion chamber, both lined with graphite liners as well as a solid fuel grain cast in paper phenolic which permits cartridge loading. The fuel grains exhibit a center-perforated geometry, having a 9.5 mm ID port. Pressure transducers permit measurement and recording of pre and post combustion chamber pressures, as well as monitor the oxygen and nitrogen purge line pressures upstream of the critical orifices. A pressure transducer was also inserted upstream of the valve in the N₂O line to measure the pressure. The system was sled-mounted on linear guide bearings to permit instantaneous thrust measurement

using a 220 N load cell located at the head end of the sled. The chamber allowed for an operational pressure limit of 13.8 MPa (2,000 psig).

Pneumatic ball valves were used to control oxygen and nitrogen purge flow during motor operation. Ignition was achieved using an electric match placed within the grain port, fired once oxidizer flow reached steady state conditions. A ten pound Nitrous Oxide Systems (NOS) cylinder was used to feed N_2O to the head end of the motor via stainless steel flex lines, with a solenoid valve to control the on and off capabilities of the N_2O . Since the equation for choked flow of an ideal gas could not be used for the N_2O , each orifice used was calibrated to give the mass flow rate of the oxidizer. A custom LabVIEW program was used for data acquisition and motor control. Data was recorded with the LabVIEW program at 1000 Hz. Oxygen flow was initiated three seconds prior to ignition to ensure steady-state conditions were achieved. Once ignited, oxygen was permitted to continue to flow for 1.1 seconds while the N_2O flow was initiated and allowed to overlap for 0.1s to ensure an oxygen rich environment, mitigating potential N_2O hard start complications. Firing with N_2O flow was permitted to continue for a predetermined duration, followed by a nitrogen purge, which quenched combustion, concluding the test run.

The oxidizer flow system was designed to permit interchanging of critical flow orifices to obtain different mass flow rates of N_2O . For the experimental matrix considered for the current work, the average oxidizer mass flux ranged from 60 to 145 $\text{kg/m}^2\text{-s}$. Not only could the orifices be changed for different flow rates, but also the fuel grain itself could be varied in length to obtain different oxidizer-to-fuel ratios. For the testing conducted, the fuel grain lengths were set at a length of 15.24 cm (6 in). A photograph and a schematic diagram of the LSHR are presented in Figure 3.6.

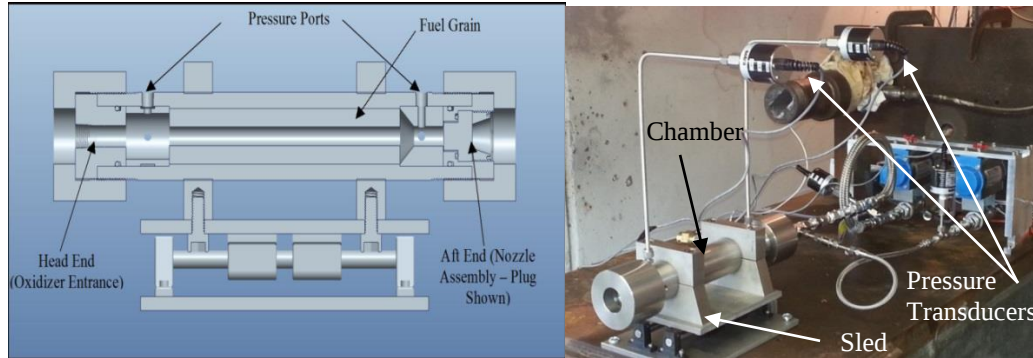


Figure 3.6: Schematic diagram of the Lab Scale Hybrid Rocket (LSHR), and an image of the assembled static-fired motor and feed system [26].

The LSHR was located in a test cell with a separate remote control area where the LabVIEW program to operate the motor was controlled. There was a Standard Operating Procedure (SOP) established for conducting motor setup and firings based on hazard analysis and experience, with an abbreviated checklist used for regular motor operations to ensure all SOP steps were followed correctly.

Penn State's HPCL utilizes a rocket motor similar to the LSHR used for hybrid fuel firings at Indian Head NSWC, called the Long Grain Center Perforated Hybrid Rocket Motor (LGCP). This system preceded the LSHR and provided guidance for the LSHR design. Risha developed the LGCP to investigate burning rates of solid fuel compositions and characterize propulsive performance, conducting experiments with GOx and HTPB-based solid fuels [4] [28] [29].

The LGCP has a 53 cm (21in) long chamber with a 38.1 mm (1.5in) ID, allowing fuel grains up to 40.64 cm (16in) in length in addition to pre and post-combustion chamber sections. Any remaining free-chamber volume is filled with graphite to reduce pressure rise time and protect the chamber wall from hot combustion products. The solid fuel grains were cast in

phenolic tubing with an OD of 38.1 mm (1.5 in) and an ID of 31.75 mm (1.25 in) with a port diameter of 6.35 mm (0.25 in).

At each end of the rocket motor, there is a piston O-ring sealed stainless steel cap. The fore-end cap houses an interchangeable injector connected to the oxidizer feed system. The cap that attaches to the aft end holds a replaceable nozzle made from graphite. Pressure taps in the pre and post combustion chamber permit chamber pressure measurement. Pressure transducers were also used upstream and downstream of flow control orifices to measure oxidizer flow rate. A schematic of the LGCP is shown below in Figure 3.7.

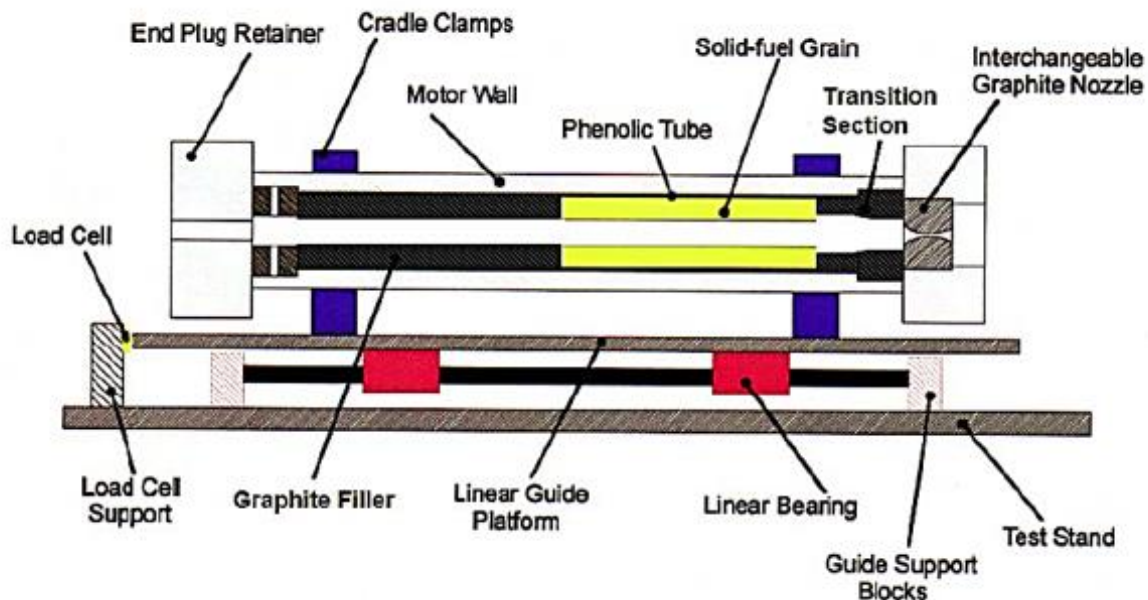


Figure 3.7: Schematic of the Long Grain Center Perforated Rocket Motor (LGCP) [4].

The LGCP stainless steel chamber was pressure tested to a pressure of 12.1 MPa (1,750psig). The firings were conducted at 4.1-5.5 MPa (600-800psig) for the tests with aluminized fuels specified by NASA. The chamber pressure was easily varied by changing the nozzle utilizing a different throat diameter; although the actual pressure achieved during a test depends on the performance of the fuel grain.

The oxidizer system was quite similar to that used for the LSHR where pneumatic ball valves were used to control the start and stop capabilities of the oxidizer. A pictured walkthrough of the oxidizer system for the LGCP can be seen in Appendix D. Below is a diagram of the GOx setup seen in Figure 3.8. The LGCP was also designed to be used with a storable liquid oxidizer such as N_2O .



As with the LSHR, the LGCP was located in a separate test cell with an SOP along with the abbreviated checklist for regular test operations to ensure all SOP steps are followed correctly, which can be seen in Appendix C.

CHAPTER 4: Experimental Results and Discussion

4.1 Counterflow Burners

The counterflow burner developed at Indian Head NSWC was used to obtain regression rates of the solid fuel pellets using gaseous N_2O and GOx . The oxidizer tube exit velocities were kept constant during each test (~ 75.59 cm/s) for both oxidizers. Aluminized HTPB solid fuels were also tested with GOx at a velocity of 75.59 cm/s at atmospheric pressure in the PCBE to observe the difference between the two systems. Summaries of the regression rate data for both oxidizers with pure HTPB as well as aluminized compositions are presented in Figure 4.1 and Figure 4.2.

As can be seen in Figure 4.1 and Figure 4.2, it is apparent that the HTPB regression rate shows a slight linear decrease with increasing aluminum for N_2O as the oxidizer, while the regression rate increases slightly with aluminum loading for the GOx . Young *et al.* and Shark *et al.* observed HTPB loaded with 10 wt% of nanoaluminum did not increase solid fuel regression rate, consistent with the results presented in Figure 4.1 which shows a decrease [19] [24]. The PCBE burn rates were much lower, although the trend was the same. The PCBE results with aluminum addition will be discussed in detail later. In general, the changes are not significant when compared to the uncertainties in the data for the H2 and H12 aluminized solid fuels up to 20 wt%.

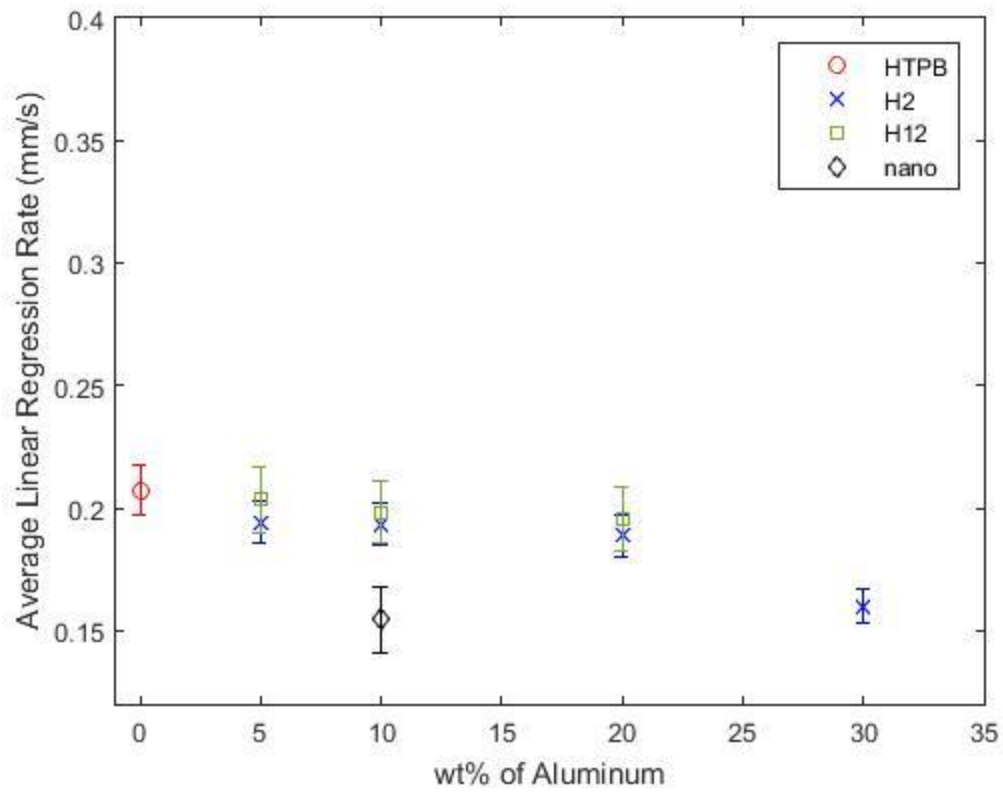


Figure 4.1: Measured regression rates for solid fuels containing up to 30 wt% H₂, H12 aluminum and nanoaluminum with N₂O at atmospheric pressure.

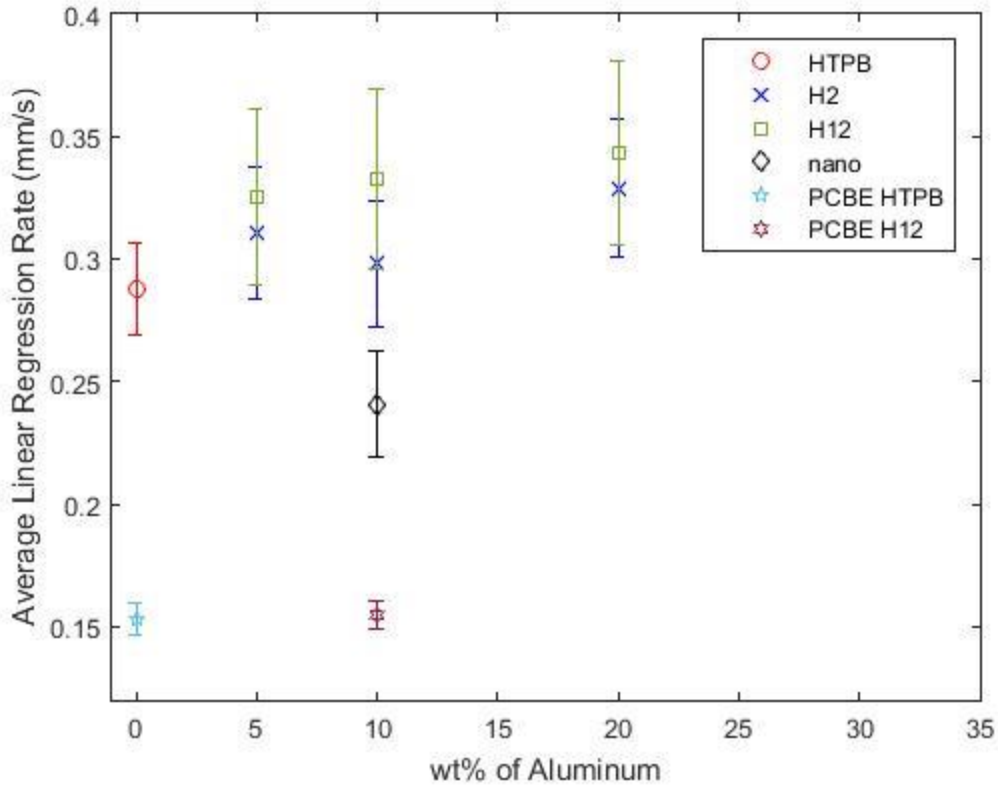


Figure 4.2: Measured regression rates for solid fuels containing up to 30 wt% H2, H12 aluminum and nanoaluminum with GOx tested in both counterflow burners at atmospheric pressure.

As discussed in section 1.1.3, as the aluminum particle size decreases (as seen with nanoaluminum compared to micron-scale aluminum), there is an increase in the regression rate. However, the nanoaluminum solid fuel regression rate shown in Figure 4.1 and Figure 4.2 is lower than all other solid fuels tested. It is unclear why this is occurring. The decrease in regression rate with nanoaluminum seemed to be counterintuitive and may be an artifact of the experiment. The same trend was seen with Young *et al.* and Shark *et al.* when they noticed that the regression rate decreased with the addition of 10% nanoaluminum compared to the baseline HTPB. The aluminum particles were observed being ejected away from the fuel surface for Shark *et al.* [19]. However, in the current study, the aluminum was observed to be collecting in

the surface melt layer, and therefore not participating in the combustion reactions above the surface.

In Figure 4.2, the regression rates obtained with the PCBE were 60% lower than the Indian Head NSWC counterflow burner. As previously discussed in sections 2.1 and 3.2.1, the strain rate has an effect on the linear regression rate; this is displayed in Figure 4.3. The strain rate was evaluated at atmospheric pressure in the PCBE, to demonstrate the effect that strain rate has on the linear regression rate.

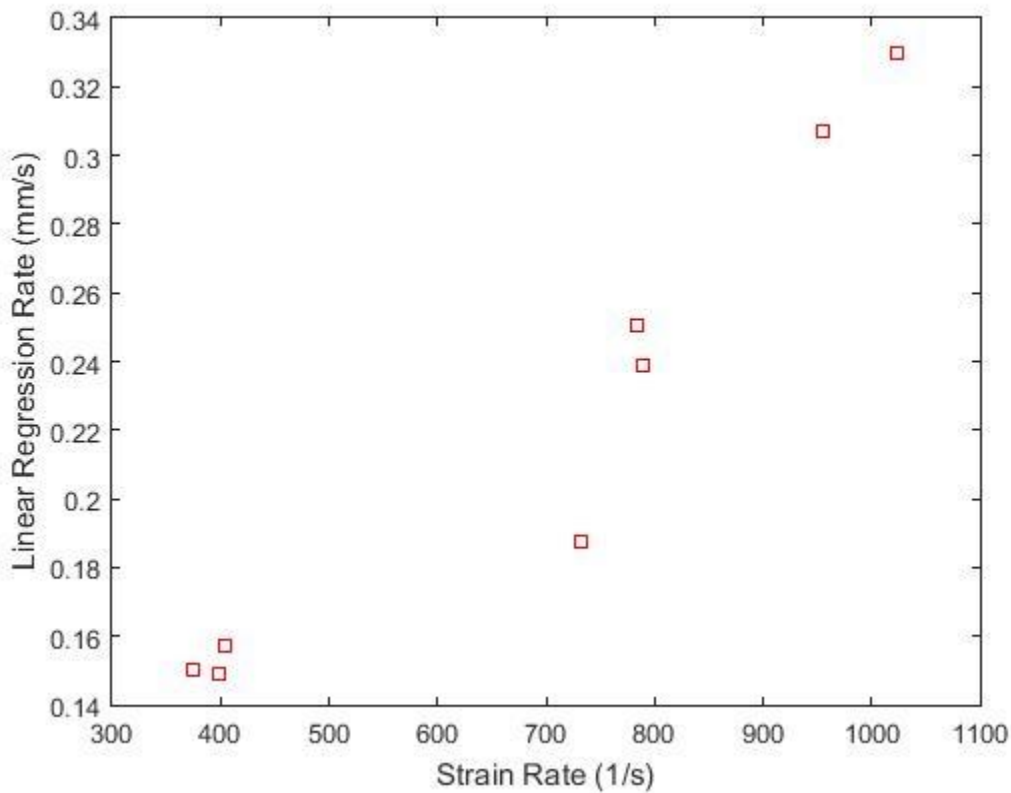


Figure 4.3: Linear regression rate as a function of strain rate for HTPB solid fuels in the PCBE at atmospheric pressure.

As the strain rate is increased, either due to a change in velocity or separation distance the regression rate increases. Since the velocity was held constant in the counterflow burner

experiments to understand the difference between the two data points obtained from the two burners, the separation distance was examined. As expected, the separation distance and the strain rate was 56% lower for the experiments conducted in the PCBE, overall causing the 60% decrease in linear regression rate. This can also be observed in Figure 4.3. At the lower strain rate, the results of the PCBE show that the larger H12 aluminum particles had essentially no effect on the solid fuel regression rate, indicating that with the H12 aluminum, it is likely that less aluminum left the surface at the lower strain rate versus the higher strain rates, due to the lower gasification velocity.

To better understand the combustion/regression rate behavior of the fuels, emission spectroscopy was conducted during the opposed flow tests at Indian Head NSWC. Spectra were collected from ~198 to 532 nm using an Ocean Optics USB 4000 spectrometer coupled to a one-inch diameter collection lens. Figure 4.4 and Figure 4.5 display the emission spectra for the 20% aluminized H12 samples for both N_2O and GOx . Emission captured at a wavelength of 431 nm, is attributed to CH produced by HTPB combustion. During this study, AlO was detected (460 and 484 nm) in all of the experiments with GOx as the oxidizer; however, no AlO emission was observed when using N_2O . Aluminum emission was also observed (394 and 396 nm) with GOx . None of the aluminized fuels combusted with N_2O therefore there was no emission corresponding to AlO or Al. Lack of AlO emission during N_2O combustion suggests the aluminum particles were not burning effectively, behaving as inert mass, absorbing energy released by solid fuel/oxidizer combustion, or not leaving the fuel surface; in any case, not contributing to the overall heat release and therefore decreasing the regression rate as seen in Figure 4.1. Thus particles, indicating AlO emission during GOx combustion, results in increased

flame temperature, which in turn increases heat feedback to the regressing fuel surface resulting in an accelerated regression rate.

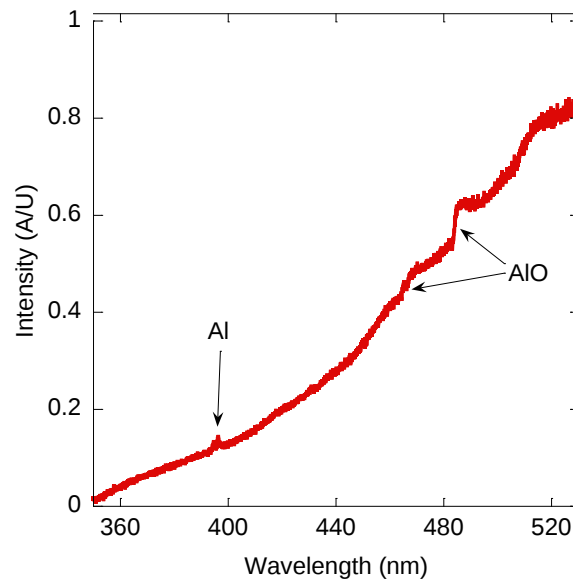


Figure 4.4: Emission spectra for HTPB fuel containing 20 wt % H12 aluminum combusted with GOx .

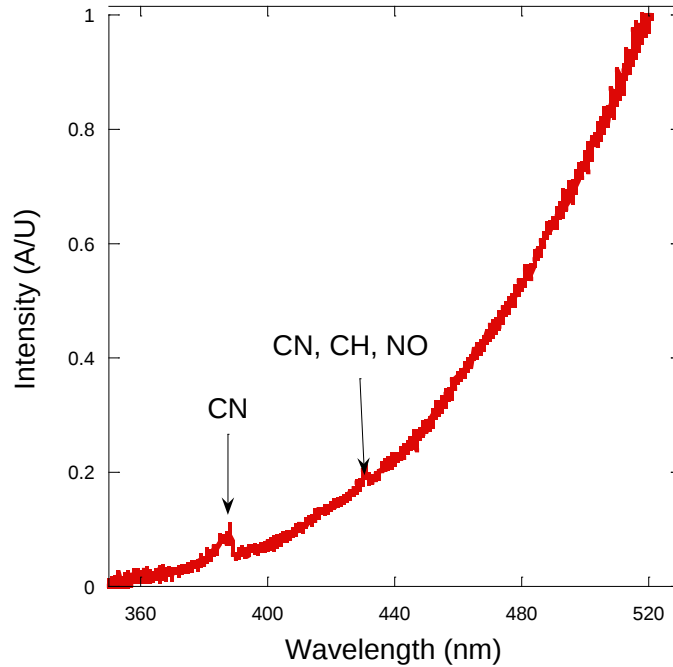


Figure 4.5: Emission spectra for HTPB fuel containing 20 wt % H12 aluminum combusted with N_2O .

Even with the slight increase in regression rate for the GOx and decrease with the N_2O , it is hard to tell if the regression rate was increasing and decreasing respectively, due to the scatter in the data. Although not statistically significant, there are opposite trends occurring with the two oxidizers; using N_2O the fuel regression rate with 20 wt% H12 decreased by 6% from the baseline HTPB, while with GOx the regression rate increases 20% between pure HTPB and 20 wt% H12.

To obtain regression rates at elevated pressures closer to those used in hybrid rocket motors, the PCBE was used. To characterize the PCBE, fuel pellets of HTPB samples were examined with GOx under varied pressure environments, and oxidizer momentum fluxes, and compared to the HTPB/ GOx data of both Risha *et al* [4] and Johansson (obtained previously using the PCBE) [6]. Each of these studies were performed with inert co-flows around both the oxidizer flow and pellet sample. Comparison of the results in the current study to previous data

provides confidence in the experimental setup and ability to obtain correct results with N_2O . Measured regression rate data as well as data obtained from Risha *et al.* and Johansson are presented in Figure 4.6 as a function of momentum flux. The momentum flux, β , is simply:

$$\beta = \rho V^2 \quad (4.1)$$

where ρ is the density, and V is the oxidizer velocity at the exit. As the oxidizer flow rate increases, the stagnation plane and therefore flame move closer to the solid fuel surface increasing heat feedback and resulting in an increase in regression rate. Figure 4.6 shows the current data matches well with published data, providing confidence in the experimental setup and operation.

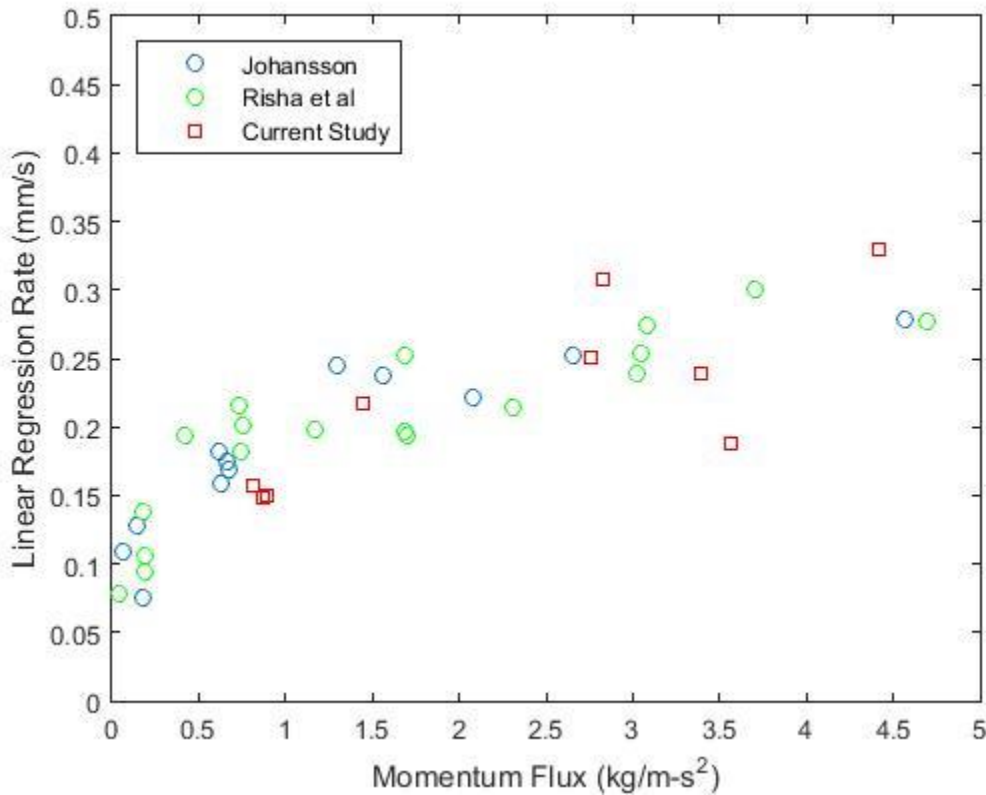


Figure 4.6: Regression rate of HTPB with GOx at various momentum flow rates, compared to published data at atmospheric pressure [4] [6].

Solid fuel regression rates are typically correlated with respect to the oxidizer mass flux or velocity, and this works fine for comparisons at a constant pressure. However, when comparing different pressures, the effect of changes in density and the resulting decrease in velocity must be taken into consideration. Therefore, for experiments at various pressures, the momentum flux of the oxidizer was kept constant to take into account the density effect as seen in Eq. 4.1. Figure 4.7 displays the results where the plotted linear regression rate for each respective pressure is an average of rates obtained from four experiments at the same condition. The uncertainty and error bars in the linear regression rate were found from the mean and standard deviation of the repeated experiments at each pressure. Again, the data in the current study showed reasonable agreement with previous data, providing confidence in the system.

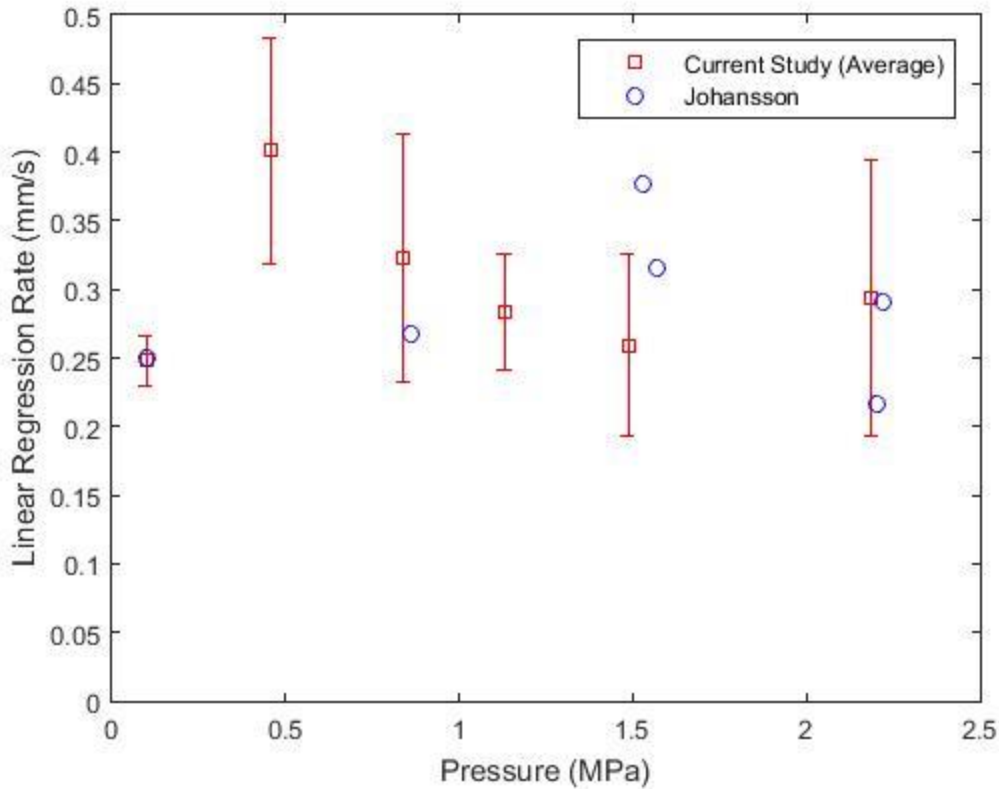


Figure 4.7: Average linear regression rate as a function of pressure for GOx in the PCBE at a constant momentum flux of $2.52 \pm 0.14 \text{ kg/m-s}^2$ compared to Johansson [6].

Figure 4.8 shows averaged linear regression rate data for pure HTPB over a range of pressures, using N₂O with a fixed momentum flux of $2.42 \pm 0.31 \text{ kg/m-s}^2$ at increasing pressure.

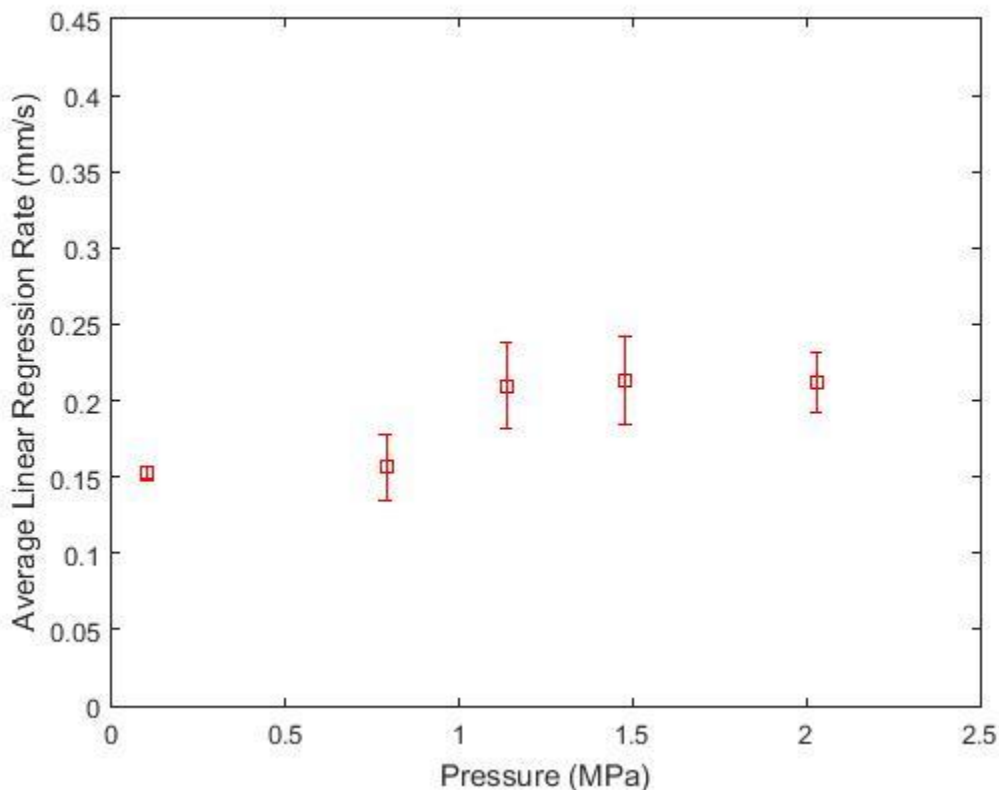


Figure 4.8: Average linear regression rate as a function of pressure for HTPB and N₂O in the PCBE at a constant momentum flux of $2.42 \pm 0.31 \text{ kg/m-s}^2$.

The linear regression rate appears to increase with increasing pressure until a plateau is observed starting at approximately 1.1 MPa (150psig). Pressure dependence of the N₂O exothermic decomposition behavior might explain the plateau behavior, therefore the N₂O decomposition is looked at in closer detail.

N₂O decomposes to form N₂ and O₂ as seen in the reaction below:



this is considered to be a unimolecular reaction. A unimolecular reaction is a chemical process under which a reactant (in this case N_2O) undergoes an isomerization or decomposition process. A unimolecular reaction must acquire significant energy before the actual reaction can occur (i.e., intermolecular energy transfer through collision) demonstrated by the equation below [23].



Where M is the third body. A unimolecular decomposition reaction in reverse is a radical-radical or radical-molecular recombination. The recombination reactions tend to slow down the reaction process playing an important role in combustion. It is interesting to note that the specific rate constant of a unimolecular reaction is both temperature and pressure dependent. This can be seen in Figure 4.9 (after a figure from Law) [23].

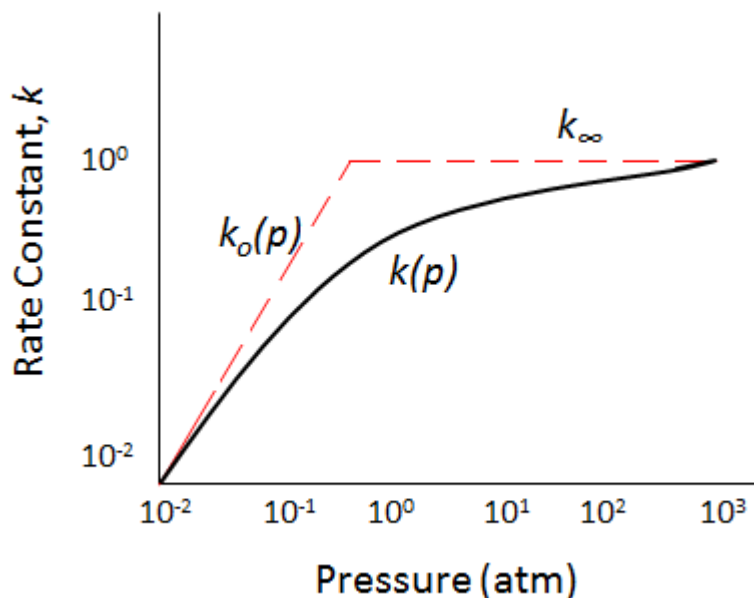


Figure 4.9: Characteristic variation of a unimolecular reaction rate constant with pressure [23].

As shown in Figure 4.9, the rate constant, k , increases with pressure for low pressures, becoming constant above a certain pressure. In going to low pressures, the reaction transitions from first to second order. The rate constant at the higher pressure region is the high-pressure

limit, k_{∞} , whereas at lower pressures, the limiting rate constant is the low-pressure limit, k_0 . In between the two limiting pressures, the effective rate constant is in the “fall-off” regime. To determine where this transition occurs for N_2O , the Lindemann Theory was used [23].

The Lindemann Theory states, “since stable molecules cannot spontaneously break up into products, the reactant must attain sufficient energy to undergo reaction.” [23]. Typically such decomposition reactions do not occur in a single step but in a series of steps, in which the first step is usually unimolecular decomposition. At higher pressures, the reaction is considered to be first order, yet as pressure decreases the rate of reaction is dependent on the rate of energization, and is proportional to the square of the concentration of reacting molecules, resulting in a second order reaction. The Lindemann Theory mechanism is shown below:



where A represents the reacting molecule, in this case, N_2O , A^* is the energized molecule, and B is the product. Applying the steady-state approximation, the three different rate constants can be found. Using the steady state analysis on A^* gives:

$$\frac{d[A^*]}{dt} = k_1[A]^2 - k_{-1}[A^*][A] - k_2[A^*] = 0 \quad (4.7)$$

the rate of reaction for the formation of product B is:

$$r_A = k_2[A^*] \quad (4.8)$$

this equation can be re-written in terms of $[A]$,

$$r_A = \frac{k_1 k_2 [A]^2}{k_2 + k_{-1} [A]} \quad (4.9)$$

where at high pressures $k_{-1}[A] \gg k_2$, therefore the rate expression can be expressed in terms of the high pressure rate constant

$$r_A + \frac{k_1 k_2}{k_{-1}} [A] = k_\infty [A] \quad (4.10)$$

which is a first order term. However, at low pressures, $k_{-1}[A] \ll k_2$, and therefore; k_{-1} may be neglected, showing that the low pressure rate constant is a second-order rate constant:

$$r_A + \frac{k_1 k_2}{k_{-1}} [A] = k_\infty [A] \quad (4.11)$$

$$r_A = k_o [A]^2 \quad (4.12)$$

so that the reaction goes from second order to first order as the pressure is increased [31].

All of the rate constants have been determined experimentally through Arrhenius rate parameters. Using Arrhenius expressions from literature, the high and low pressure rate constants can be determined.

$$k_o = A_o T^{\beta_o} e^{\frac{-E_o}{RT}} \quad (4.13)$$

$$k_\infty = A_\infty T^{\beta_\infty} e^{\frac{-E_\infty}{RT}} \quad (4.14)$$

The rate constant at any pressure is given by:

$$k = k_\infty \left(\frac{P_r}{1 + P_r} \right)^F \quad (4.15)$$

where P_r is the reduced pressure:

$$P_r = \frac{k_o [M]}{k_\infty} \quad (4.16)$$

In Eq. 4.16 $[M]$ is the concentration of the mixture, including any enhanced third body efficiencies. These equations are used in CHEMKIN for unimolecular reactions [32].

From the literature, the Arrhenius expressions for N_2O were found and the third body considered was N_2 . Using the Arrhenius expressions, the pressure that corresponds to the center of the fall-off is, 0.778 MPa (114 psi). This pressure appears to correspond with the pressure at which the regression rate becomes independent of pressure (approximately 1.1 MPa) in the PCBE. Using the Lindemann Theory, however, is limiting since it does not take into account two major factors:

1. Energy dependence of activation for the bimolecular step.
2. The unimolecular step does not take into account that a unimolecular reaction involves one particular form of molecular motion [33].

Considerable research has been conducted on low pressure decomposition of N_2O , with only a couple references for pressures above 1 atm. Kalback determined that the fall-off pressure at a temperature of 605 °C was found to be around 0.896 MPa (130 psi) [31]. Therefore, it is evident that when HTPB reacts with N_2O , a pressure dependence on the regression rate may occur, due to the behavior of the unimolecular reaction of N_2O . Consistent with the results of Kalback, above the observed fall-off region near 0.896 MPa the regression rate became independent of pressure.

It should also be noted that as the pressure is increased from 0.101 MPa to 1.827 MPa, the Reynolds number changes from 1000 to 5000 in the oxidizer tube. With the oxidizer tube length being 10 times the diameter, there is sufficient amount of length for the flow to transition to turbulent. Consequently, as the pressure is increased, there may also be an effect of turbulence in the reaction rate. However, although the flow may be turbulent at the exit of the oxidizer

nozzle at higher pressures, the decay of the turbulence as the flow exits the nozzle and enters the reaction zone may be considerably less due to the decrease in velocity and increase in temperature, increasing viscosity. Therefore, the flow effects were not taken into consideration.

The results from the counterflow burner experiments indicate some important observations.

1. The regression rate with N_2O as an oxidizer appears to be 50% lower than the regression rate with O_2 as the oxidizer.
2. The regression rate, or equivalently the rate at which gas evolves from the surface, is important to the entrainment of the aluminum particles. At the lowest regression rates, which were mostly associated with N_2O as the oxidizer or low strain rate experiments, the gas evolution rate was not sufficient to overcome the surface forces holding the aluminum, and consequently, it was difficult to entrain the aluminum.
3. Some pressure dependence may be observed in the regression rate of HTPB when N_2O is the oxidizer, which may be related to the fall-off behavior of the N_2O decomposition reaction.

4.2 Hybrid Rocket Motors

Two hybrid rocket motors, the LSHR and LGCP, were used to conduct static-fired experiments to study the baseline HTPB and aluminized HTPB fuel grains. The primary focus of the motor experiments was to determine regression rates and combustion efficiencies of the aluminized fuel compositions with N_2O and GOx under realistic rocket motor pressure and flow operating conditions. N_2O motor firings were conducted using the LSHR, while LGCP firings were conducted with GOx .

Analysis of the fuel grains was done using averaging techniques that are commonly performed when determining the performance of a rocket motor. The initial and final fuel grain mass and port diameter were recorded for each experiment, and used in calculating the performance parameters. The average regression rate, $\bar{\dot{r}}$, was determined from the difference in initial and final port radius, r_i and r_f , respectively, divided by the burn duration, t_b . This is shown below:

$$\bar{\dot{r}} = \frac{r_f - r_i}{t_b} \quad (4.17)$$

the burn duration was determined from the pressure-time trace recorded during a motor firing, an example is provided in Figure 4.10.

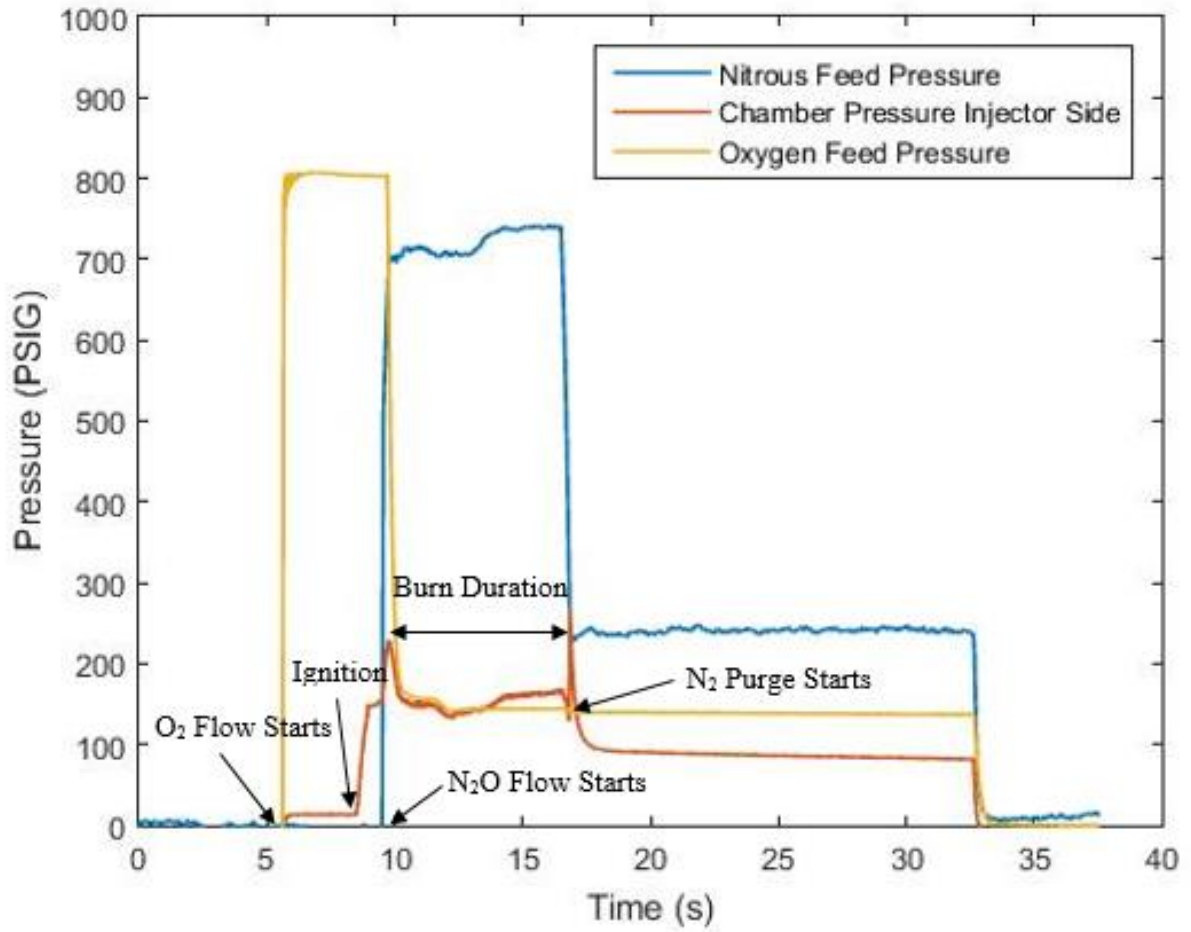


Figure 4.10: Pressure-time trace for a typical LSHR firing. Pressure time trace provided is for a 10 wt% H₂ aluminized fuel grain with N₂O at an average chamber pressure of 1.17 MPa (170 psi).

As discussed in the literature review, the regression rate is normally correlated to an average oxidizer mass flux, $\bar{G}_{ox}$, which is the average mass flow rate of the oxidizer, $\bar{m}_{ox}$, divided by the average port area during the test.

$$\bar{G}_{ox} = \frac{\bar{m}_{ox}}{\pi(r_f - r_i)^2} \quad (4.18)$$

The combustion efficiency, η , is found by comparing the experimental characteristic velocity, c^* , to the theoretical value, c^*_{ideal} , found from NASA CEA2 code. The experimental

characteristic velocity as shown in Eq. 4.19, is determined from the combustion chamber pressure, $\bar{P}_c$, which is the average value measured from the experiment at steady state conditions, A^* is the nozzle throat area and $\bar{m}_f$ the average fuel flow rate. The combustion efficiency is given by Eq. 4.20.

$$c^* = \frac{\bar{P}_c A^*}{\bar{m}_f + \bar{m}_{ox}} \quad (4.19)$$

$$\eta = \frac{c^*}{c^*_{ideal}} \quad (4.20)$$

The average fuel flow rate is determined by taking the difference in the initial and final mass of the fuel grain, M_i and M_f , respectively, and dividing it by the test duration, as shown below.

$$\bar{m}_f = \frac{M_i - M_f}{t_b} \quad (4.21)$$

Using these equations, the average regression rate and average combustion efficiency were found for each rocket motor firing.

4.2.1 Lab Scale Hybrid Rocket Motor

The LSHR was used to obtain regression rate data for HTPB fuels with N_2O . The before and after measurements of the fuel grains along with the pressure time trace allowed the regression rates and combustion efficiencies to be calculated. Figure 4.11 shows a typical LSHR motor firing. A set of pressure-time traces for each experiment allowed for the determination of the run duration, pressure in the lines corresponding to an oxidizer flow rate, and chamber pressure. A typical LSHR pressure time trace, shown previously, is provided in Figure 4.10. In Figure 4.10, GOx flow was initiated prior to ignition to achieve a rich oxygen environment for 1.1 s, with a 0.1 s overlap between the GOx and N_2O flows to ensure ignition. The N_2O was

flowed for seven seconds, after which the valve is then shut. A flow of nitrogen was then introduced to quench any reactions and to purge the system for a duration of 20 s. The test duration consisted of seven seconds of N_2O flow to ensure that web thickness remained for post-test measurements, targeting an average oxidizer mass flux of $60 \text{ kg/m}^2\text{s}$ over this duration using a 0.736 mm (0.029 in) choked flow orifice.

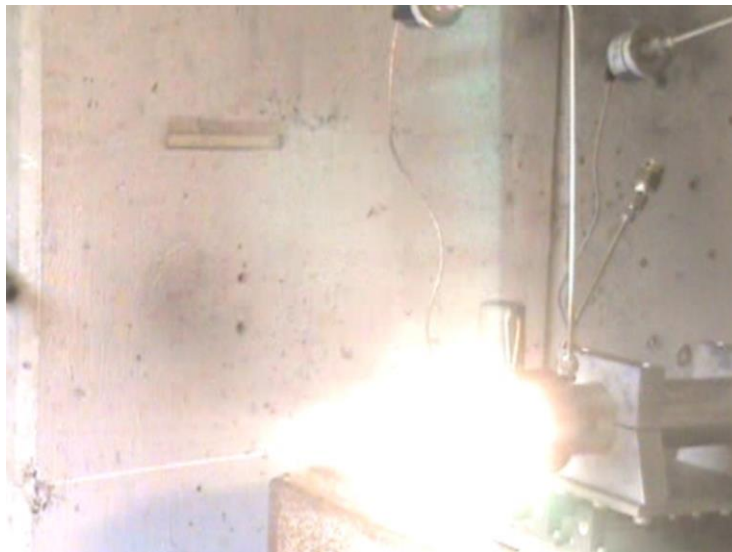


Figure 4.11: Photograph of a typical LSHR test firing for a 10 wt% H_2 aluminized fuel grain with N_2O at an average chamber pressure of 1.17 MPa (170 psi) and constant oxidizer mass flow rate.

Three fuel grains of each HTPB based fuel grain composition, (as given in Table 3.2) were evaluated. Multiple firings for each HTPB solid fuel composition were run at identical conditions (same oxidizer mass flow), the results were then averaged for each HTPB solid fuel composition and are shown in Figure 4.12. Regression rates of pure HTPB grains fired with N_2O are in reasonably good agreement with values obtained from literature (0.78 mm/s for an oxidizer mass flux of $60 \text{ kg/m}^2\text{s}$) [34]. The effect of additives can be observed in the same figure in which regression rates of HTPB grains containing aluminum powders are compared to pure HTPB, all burned with N_2O . The average regression rate is reported as a function of the size of

the aluminum particles. Tests carried out with the addition of particle loaded HTPB grains prove positive influence of the additives on regression rate. The average regression rate increased by 15% with the addition of 10 wt% H2 and H12 aluminum to HTPB solid fuel. However, there is very little effect seen with the different size aluminum particles (H2 and H12). This may be because the difference in particle sizing is too small to have a significant change in the regression rate. The increase in regression rate is in good agreement with the literature (average oxidizer mass flux of $65 \text{ kg/m}^2\text{s}$ resulting in a regression rate of around 0.91 mm/s for micro sized aluminum) [34].

Nanoaluminum fuel grains were manufactured to investigate particle size effects on the regression rate, however upon making the nanoaluminum fuel grains, production issues were encountered and they could not be fired. The high viscosity of the binder/nanoaluminum mixture, resulting from the high surface area of the nano particles, presented issues when the nanoaluminum fuel grains were cast. Upon inspection, the fuel grains had air entrapped after curing, causing air pockets to remain in the solid fuel grains, which rendered them unsuitable for motor firings.

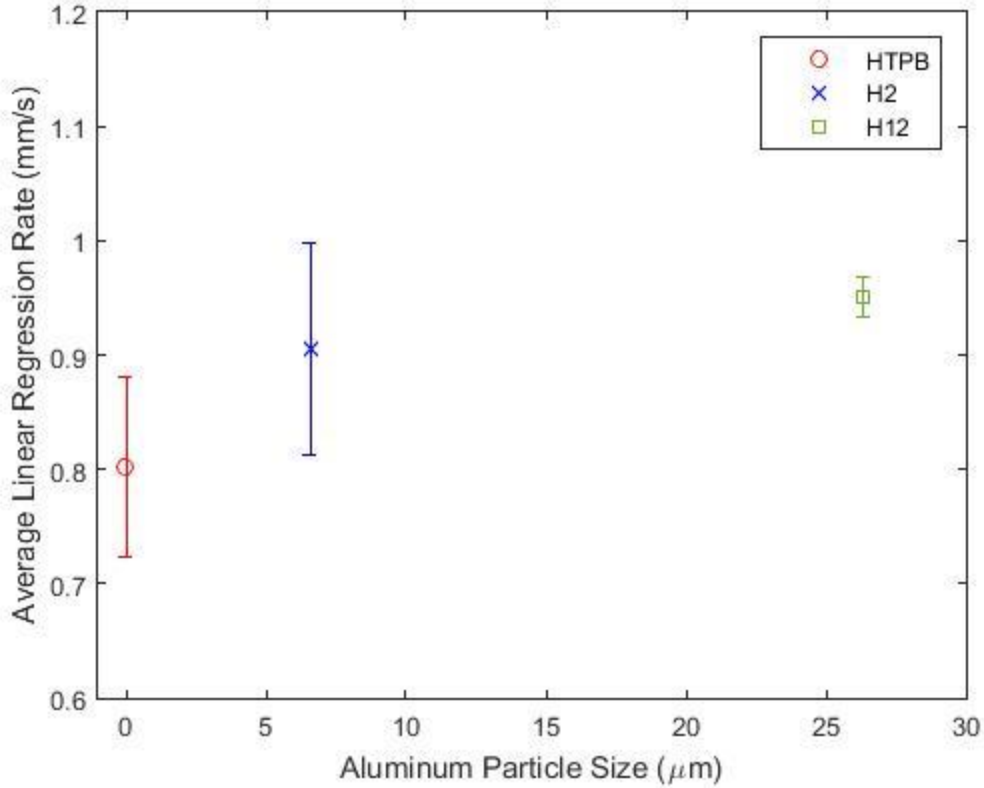


Figure 4.12: Regression rate as a function of aluminum particle sizing at 10 wt% loading in the LSHR with N₂O at an average chamber pressure between 1.17-1.37 MPa (170-200 psi) and a constant oxidizer mass flow rate.

In Figure 4.12 the regression rate improved with H12 aluminum, therefore this formulation (FG3) was further investigated using different oxidizer mass fluxes to obtain an empirical regression rate correlation. The empirical equation is governed by

$$\dot{r} = a \bar{G}_{ox}^n \quad (4.22)$$

where the regression rate is in mm/s, $\bar{G}_{ox}$, is the average oxidizer mass flux in g/cm²s, and a and n are empirical coefficients. As seen in Figure 4.13, where the regression rate and oxidizer mass flux were plotted on a logarithmic scale, the FG3 containing 10 wt% H12 particles follows the empirical power law formula, displayed in Eq. 4.23:

$$\dot{r} = 0.5049G_{ox}^{0.349} \quad (4.23)$$

Doran *et al* studied HTPB combusted with N₂O providing an empirical correlation shown in Eq. 4.24 [35].

$$\dot{r} = 0.417G_{ox}^{0.347} \quad (4.24)$$

Using the empirical correlation of Doran *et al.* with an average oxidizer mass flux used in the rocket motor firings (6 g/cm²s) corresponds to a 0.78 mm/s linear regression rate for pure HTPB. With an average linear regression rate for pure HTBP in the LSHR of 0.81 mm/s, shows that the correlation corresponds well to the experimental firings in the LSHR, therefore can be used as a comparison to the FG3 correlation. There was an increase seen with the exponent a , for the aluminized grains with the same slope, n , showing an increase in the regression rate and regression rate empirical correlation compared to that of pure HTPB.

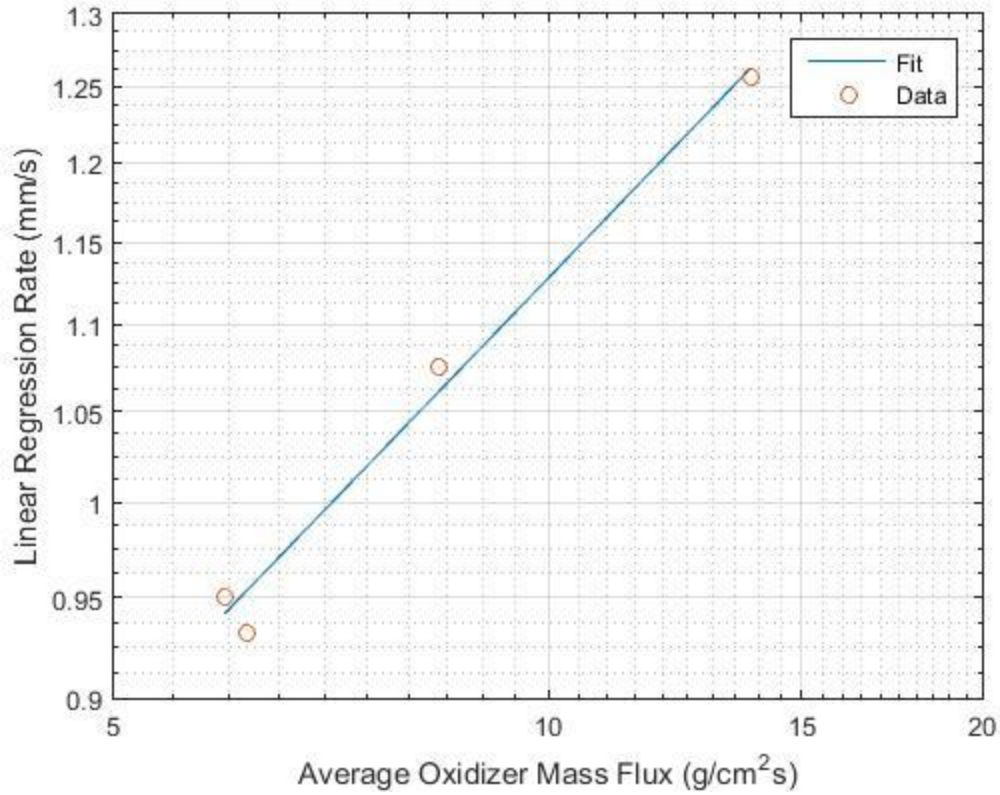


Figure 4.13: Empirical regression rate correlation for 10 wt% H12 HTPB fuel grain in the LSHR with N₂O.

Risha focused on HTPB and aluminized fuel with GOx using the LGCP at the HPCL and found an empirical correlation with pure HTPB and GOx, shown in Eq. 4.25 [4]. Aluminized HTPB was also tested in the LGCP at a loading of 13 wt% using NTECH-50, this correlation is shown in Eq. 4.26.

$$\dot{r} = 0.241 G_{ox}^{0.647} \quad (4.25)$$

$$\dot{r} = 0.244 G_{ox}^{0.710} \quad (4.26)$$

It is evident that the exponent for GOx is 59% higher than that of pure HTPB with N₂O. Although the slope may be higher with GOx, the pre-exponential factor is 50% lower compared

to N_2O . This increase in the pre-exponential factor causes a slight increase in regression rate over GOx systems below an oxidizer mass flux of $14 \text{ g/cm}^2\text{s}$.

Although the regression rate increased with particle size at the 10 wt% loading, the average thrust and average chamber pressure stayed relatively constant as shown in Figure 4.14. This could be occurring due to either low combustion efficiency or nozzle erosion. However, upon looking at Figure 4.15, the calculated combustion efficiency was not low, nor did it change drastically between the pure HTPB and aluminized grains. The average nozzle throat area pre and post-test was used to determine the combustion efficiency. Using an average nozzle throat area reduces the error associated with the nozzle erosion, therefore, it is unclear why the chamber pressure or combustion efficiencies for the three fuel grain compositions are alike.

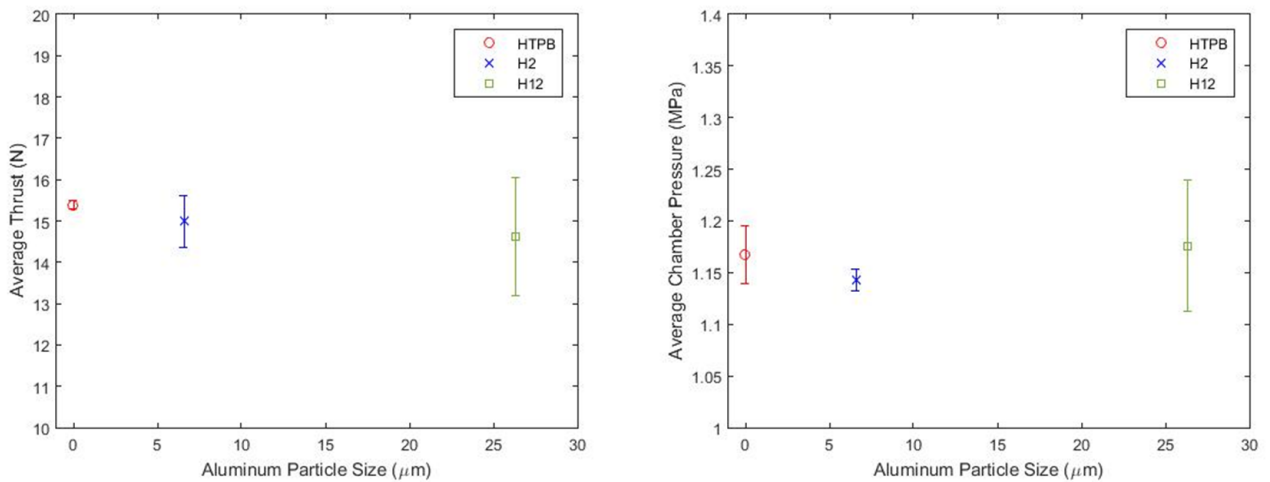


Figure 4.14: Thrust and chamber pressure as a function of aluminum particle sizing at 10 wt% loading in the LSHR with N_2O .

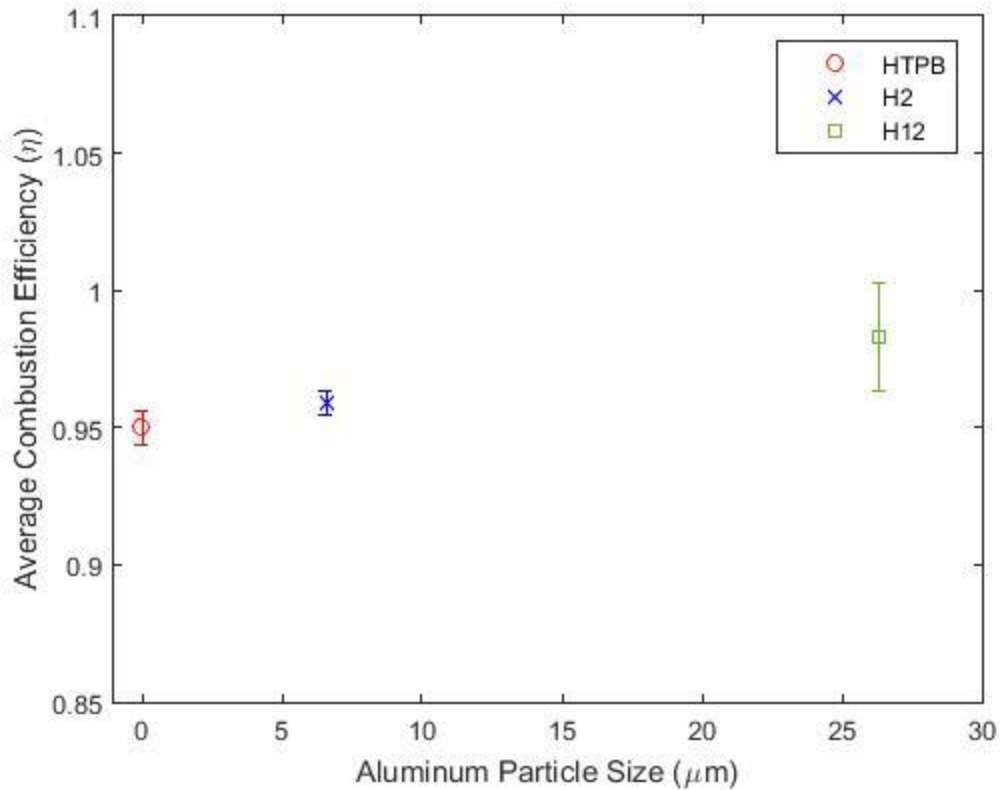


Figure 4.15: Average combustion efficiency for fuel grains fired in the LSHR as a function of aluminum particle sizing at 10wt% loading in the LSHR with N_2O .

The results from the hybrid rocket motor experiments indicate some important observations.

1. The regression rates with the aluminized HTPB fuel grains proved to be 15% higher than pure HTPB at an average oxidizer (N_2O) flux of $60 \text{ kg/m}^2\text{s}$. The 10 wt% H12 (FG3) aluminized fuel grain obtained a similar exponent to pure HTPB with N_2O , but a higher pre-exponential factor compared to Doran *et al*.
2. There was no significant difference between the performance of the H2 and H12 aluminized fuel grains, indicating that the difference in size of the H2 and H12 aluminum particles were insignificant.

3. The thrust, chamber pressure, and combustion efficiency of the three fuel grain compositions were similar. This can be attributed to the nozzle erosion during the firings.

To obtain a comparative baseline between GOx and N₂O using aluminized HTPB, NASA supplied 18 and 40% aluminized HTPB grains to conduct static fired experiments at the HPCL using GOx. These grains were provided for analysis using the LGCP to determine the behavior of high aluminum content HTPB grains with GOx. However, the grains provided during the period of this overall study all had considerable internal flaws that resulted in non-uniform burning behavior, and therefore did not generate useful data for comparison with N₂O performance with similar highly loaded fuel formulations. The overall experimental approach and inspection of the high aluminum content fuel grains is discussed in Appendix E.

CHAPTER 5: Theoretical Method of Approach

A computational model was developed to attain an understanding of the flame structure and in particular, the effect of pressure on the HTPB regression rate. To create this model CHEMKIN 10141, CHEMKIN PRO and Octave 4.0, an open source alternative to MATLAB, were used. Model input data was obtained from the opposed flow experiments and from the literature, in particular for development of the reaction mechanism. With all the input data, the species and energy equations for describing the counterflow geometry were solved to determine the burning rate, as well as the species, temperature, and heat release profiles along the stagnation streamline. The trends of the model were then compared with the experimental results.

5.1 Model Development

The regression rate for the opposed flow flame in the counterflow burner was measured using a spring-loaded LVDT which maintained the location of the fuel surface in the same position. Therefore, it can be treated as a stationary surface with steady flow of gas reacting at the surface corresponding to the burning rate. This burning of the solid fuel can be broken into different regions of interest mainly above the fuel surface.

The solid fuel is at ambient temperature prior to ignition, where at the time of ignition, heat feedback from the flame starts to increase the surface temperature to the decomposition temperature of HTPB. A melt layer begins to form, and once the temperature reaches approximately 500 K, the surface starts to degrade and pyrolyze over a limited range of temperatures [36]. This solid fuel pyrolysis creates a gas-phase region above the molten fuel surface that combines with the oxidizer, forming a diffusion flame where chemical reactions generate heat and a visible flame, as depicted in Figure 2.1.

To capture important phenomena while simplifying the calculations as much as possible to aid in implementation, the model was divided into two parts. The first part was the condensed phase model, modeled in Octave, which considered the pyrolysis of the solid HTPB. The second part was the gas-phase model, analyzed with CHEMKIN OppDiff, which took into account the combustion kinetics and the gas-phase flow field.

The system modeled in this study is the regression of HTPB held in a stainless steel pellet holder with an axially impinging oxidizer flow. The assumptions made while developing this model were that the oxidizer velocity profile was uniform and the heat loss through the walls of the pellet holder was small and therefore neglected. To start the model development, physical and thermal properties need to be known. These properties were either measured, calculated, or determined from the literature. Utilizing these properties a condensed-phase model, in Octave, was coupled with CHEMKIN's OppDiff gas-phase solver.

5.1.1 Condensed-Phase Model

To implement the CHEMKIN and Octave codes, the actual decomposition process of the HTPB fuel must be understood. The energy required for HTPB decomposition and pyrolysis results from heat transfer from the gas-phase. The heat feedback from the flame to the fuel surface raises the fuel surface temperature to the depolymerization temperature. Pyrolysis reactions occur in the pyrolysis (melt) layer forming gas-phase products which continue to undergo oxidative pyrolysis as they are transported to the diffusion flame. Figure 5.1 below shows a temperature distribution zone of a hybrid fuel grain.

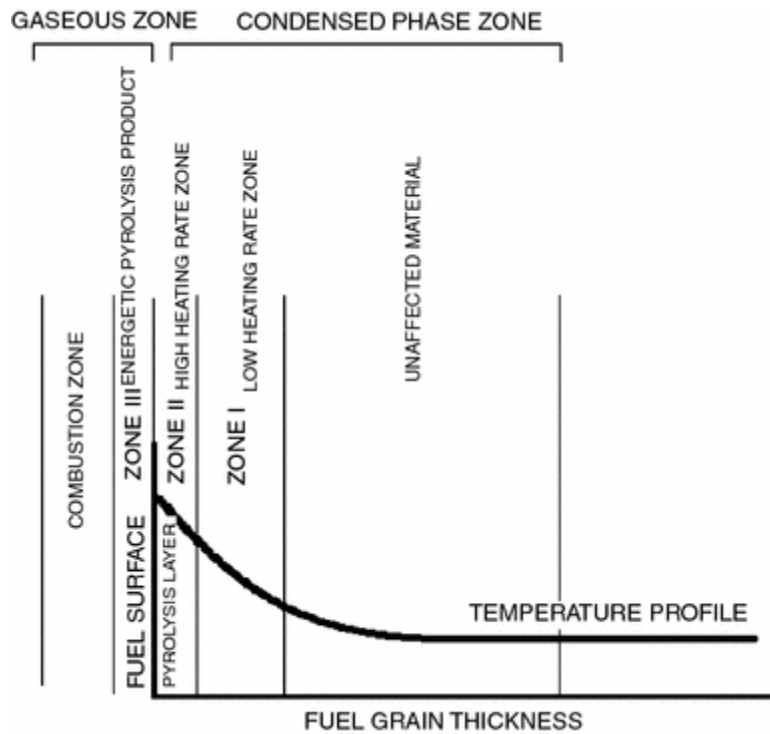


Figure 5.1: Temperature distribution zone of a hybrid fuel grain [37].

In the gas-phase reaction zone, the pyrolysis products heat up to the flame temperature mainly by heat transfer from the combustion zone [37]. The pyrolysis of HTPB has been studied by Chiaverini *et al.* in lab scale experiments using a constant temperature flash pyrolyzer furnace coupled to a gas chromatograph-mass spectrometer for species identification and quantification [36]. These experiments have provided data on pyrolysis rates as a function of temperature as well as the major decomposition products, given by Table 5.1.

Table 5.1: Pyrolysis behavior of hybrid rocket solid fuels (HTPB) under rapid heating conditions [36].

Major pyrolysis product species (Mi) chemical formula	500 °C	600 °C	700 °C	800 °C
Ethene, C ₂ H ₄		5.59	3.05	6.58
Propene, C ₃ H ₆			4.9	10.99
1,3-Butadiene, C ₄ H ₆	77.4	89.06	66.1	41.07
3-Pentene-1-yne, C ₅ H ₆			9.2	10.28
Benzene, C ₆ H ₆			10.3	22.02
Toluene, C ₇ H ₈			6.41	9.06
4- Vinyl-cyclohexene, C ₈ H ₁₂	22.6	5.35		

In the present model, the condensed-phase reaction was assumed to occur only at the interface (solid surface) separating the gas and condensed phases. The control volume (CV) in this case is then taken from below the thermal wave in the HTPB to directly above the surface as shown in Figure 5.2.

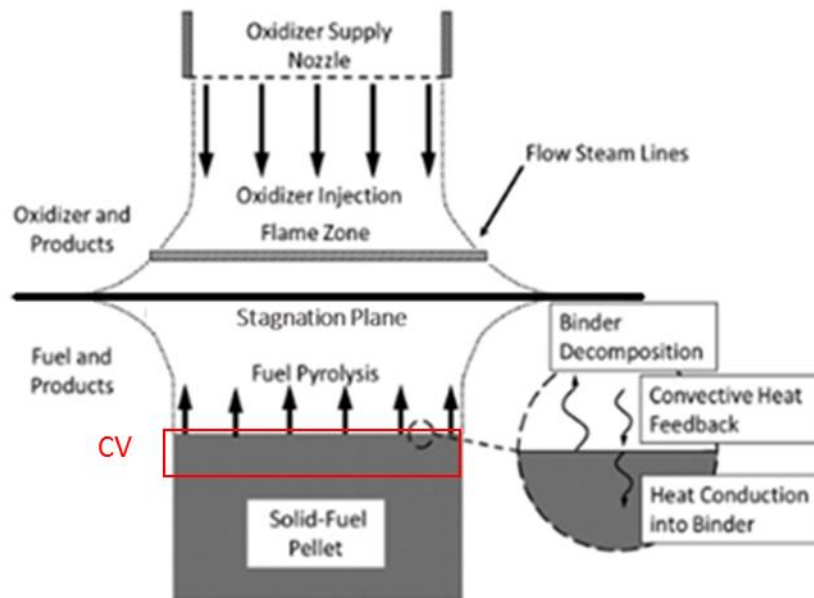


Figure 5.2: Control volume used for Octave modeling.

This treatment allows the burning surface to be considered as stationary with unreacted HTPB entering the bottom of the CV at a velocity equal to the burning rate. This model resembles that of earlier research by Boyer on liquid nitromethane, which only involved a phase change at the interface [38]. The governing equations used are as follows:

For steady state, one-dimensional flow the mass balance is

$$\dot{m} = \rho_s U_s A_s = \rho_g U_g A_g \quad (5.1)$$

for the HTPB pellet combusted using the counterflow burner experiment, the regressing surface area is constant. CHEMKIN uses an input of either mass flow or velocity, which is equivalent to the velocity at which the gas-phase pyrolysis species leave the CV, also known as surface “blowing”. Therefore the continuity equation can be reduced to

$$\frac{\dot{m}}{A} = \rho_s \dot{r} = U_g \rho_g \quad (5.2)$$

momentum in this region is neglected, assuming inviscid, isobaric flow with no body forces. The energy balance, therefore, can be written as:

$$\dot{m}h_i - \dot{m}h_g + \dot{Q}_{cond} + \dot{Q}_{rad} + \dot{Q}_{reac} = 0 \quad (5.3)$$

$\dot{Q}_{cond}$ is the heat conducted into the solid fuel at the surface (control volume), $\dot{Q}_{rad}$ is the heat transfer caused by radiation, and $\dot{Q}_{reac}$ is the energy released, or consumed, by chemical reactions taking place to pyrolyze the HTPB. $\dot{Q}_{rad}$ however, is neglected since there are no metal particles in the fuel, and it has been found in the literature that $\dot{Q}_{rad}$ for non-metalized fuels amounts to 5 to 10% of the total heat transfer [39] [40]. Chiaverini concluded that radiation in HTPB GOx systems could play a role in the regression rate and pyrolysis of the HTPB, however this was due to soot formation [41]. In the counterflow burner, there was not a significant amount of soot present to cause this radiation to factor into the energy equation. Radiant heat transfer

also tends to act as a self-regulating phenomenon. It increases solid-fuel pyrolysis, but this reduces convective or conductive heat flux by causing additional surface blowing pushing the diffusion flame further from the surface, overall diminishing the increase in blowing [41].

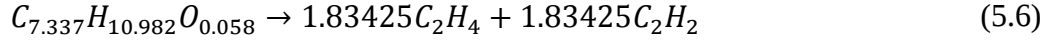
Using the assumptions provided, the energy balance can be simplified to:

$$\dot{Q}_{cond} = \dot{m}h_g - \dot{m}h_i - \dot{Q}_{reac} \quad (5.4)$$

This equation was solved by determining the enthalpy change between a point well below the surface where the temperature remained at the initial temperature and a point just above the surface where the fuel is now in the gas phase at the assumed surface temperature. The enthalpy at the initial and final phase was determined by the integral of the specific heat as a function of temperature. The heat of reaction was determined from a stoichiometric balance for the overall pyrolysis reaction for the HTPB-C₂H₄/C₂H₂ system. In Table 5.1, 1,3-butadiene is the major product from the pyrolysis of HTPB at the respective temperatures. Chambreau *et al* claimed that 1,3-butadiene decomposes to ethene (C₂H₄) and acetylene (C₂H₂), as described in the equation below [42].



With the majority of the pyrolysis of HTPB comprising of 1,3-butadiene, the decomposition products ethene and acetylene were chosen as the products of the overall decomposition reaction. Ethene and acetylene were utilized and not 1,3-butadiene because of the size and limitations of the reaction mechanism, which will be discussed later. Since HTPB only has 0.058 moles of O₂ per mole of HTPB, oxygen was omitted from the product side. Thus the overall reaction was assumed as:



and with a simple atom balance, the number of moles was determined as shown above.

From the stoichiometric coefficients and the heat of reaction, the heat of pyrolysis was determined and shown in Eq. 5.7.

$$Q_{reac} = \Delta H_{products} - \Delta H_{reactants} \quad (5.7)$$

where $\Delta H_{products}$ is found from the standard enthalpy of formation, $\Delta \dot{H}_f(products)$, and the stoichiometric coefficients, Δv_p , from the products determined using the balanced equation given below:

$$\Delta H_{products} = \sum \Delta v_p \Delta \dot{H}_f(products) \quad (5.8)$$

the same equation is then used to determine the $\Delta H_{reactants}$ for the reactants.

5.1.2 Gas-Phase Solver

The gas phase region above the surface of the solid HTPB was modeled as one-dimensional, steady state, axisymmetric, isobaric flow due to the conditions of an opposed flow flame. The equations that govern the gas-phase region are shown below:

Conservation of Mass:

$$\frac{d}{dx}(\rho u) + \frac{1}{r} \frac{d}{dr}(\rho v r) = 0 \quad (5.9)$$

where u and v are the axial and radial velocity components and ρ is the mass density.

Conservation of Species:

$$\rho u \frac{dY_i}{dx} + \frac{d}{dx}(\rho Y_i V_i) = \dot{\omega}_i \quad (5.10)$$

where Y_i is the species mass fraction and $\dot{\omega}_i$ is the species production rate.

Conservation of Energy:

$$\rho c_p u \frac{dT}{dx} = \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) - \sum_{i=1}^N \left(\rho Y_i V_i c_{pi} \frac{dT}{dx} \right) - \sum_{i=1}^N \dot{\omega}_i h_i \quad (5.11)$$

where c_p is the specific heat and λ is the thermal conductivity. The specific enthalpy, h_i , is a combination of sensible enthalpy and heat of formation of that particular species. This is shown below:

$$h_i = h_{fi}^o + \int_{T_{int}}^T c_{pi} dT \quad (5.12)$$

with the diffusion velocities given by either the multicomponent formulation

$$V_N = \frac{1}{X_N \bar{W}} \sum_{j=1}^N W_j D_{Nj} \frac{dX_j}{dx} - \frac{D_N^T}{\rho Y_k T} \frac{1}{dx} \frac{dT}{dx} \quad (5.13)$$

or the diffusion velocity can be mixture-averaged, shown below

$$V_N = -\frac{1}{X_N} D_{Nm} \frac{dX_N}{dx} - \frac{D_N^T}{\rho Y_k T} \frac{1}{dx} \frac{dT}{dx} \quad \text{where } D_{Nm} = \frac{1-Y_N}{\sum_{j=N}^N X_j / D_{jN}} \quad (5.14)$$

where D_{jN} , D_{Nm} and D_N^T are the multicomponent, mixture averaged, and thermal diffusion coefficients, respectively. The mixture averaged diffusion velocity was used in the current study.

All of these equations have already been implemented into the OppDiff driver code for CHEMKIN [43]. The flow diagram for the OppDiff driver code for CHEMKIN is shown in Figure 5.3.

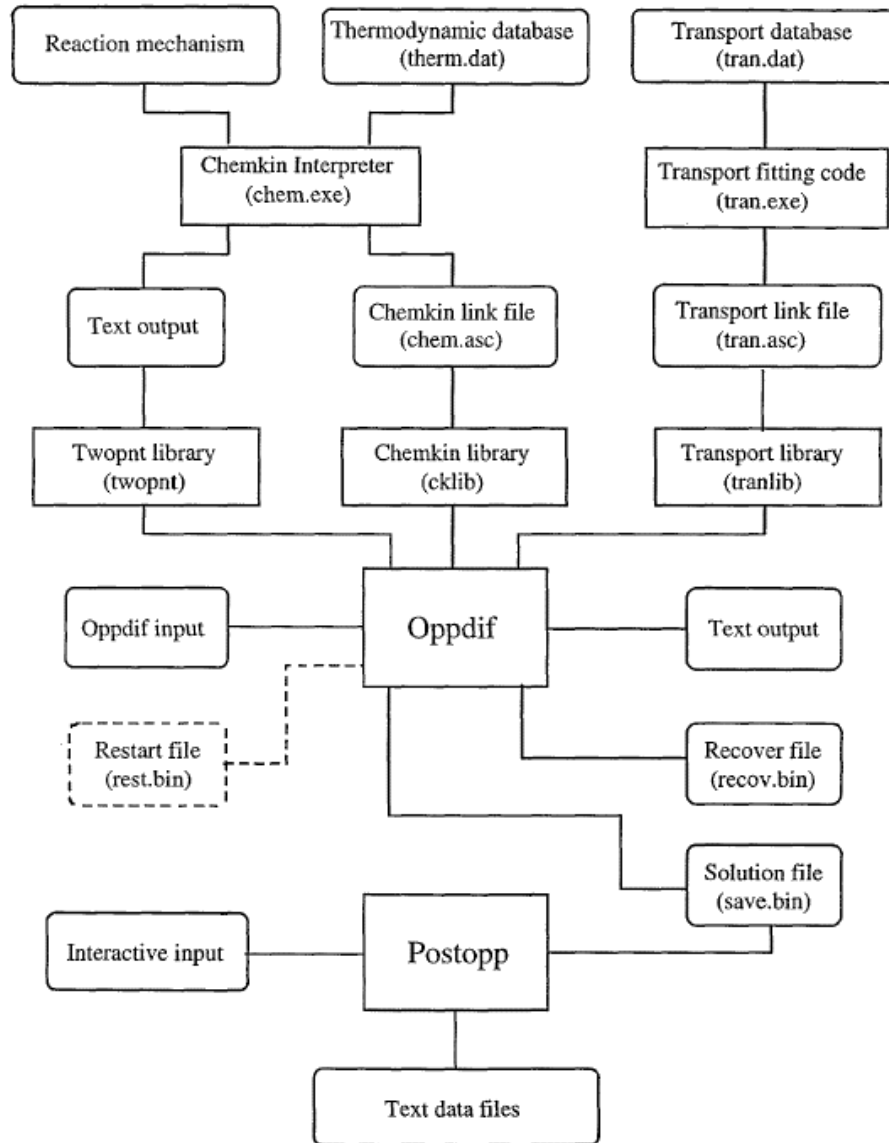


Figure 5.3: OppDiff program for computing opposed-flow diffusion flames [43].

To use CHEMKIN, the user must specify certain parameters for the given OppDiff code such as: reaction mechanism, thermodynamic properties, and transport properties, which are preprocessed for OppDiff (Chemkin, transport, and Twopt). OppDiff then reads an input, which specifies a particular problem written in a keyword format, and then outputs the solution either in a text or binary file which then can be saved and used for post-processing.

5.1.3 Solution Coupling and Code Structure

To determine the HTPB burning rate, the condensed phase model was loosely coupled to the gas-phase model, and the solutions iterated until the coupling conditions matched within a specified tolerance. Convergence was achieved by setting the mass, species, and energy fluxes at the boundary equal. The surface temperature was *a priori* chosen and kept constant. The energy from the heat flow due to conduction into the condensed phase was determined from the temperature gradient just above the surface. This is shown below.

$$T_s = T_g \quad (5.15)$$

$$\frac{\dot{Q}_{cond}}{A} = k_g \frac{dT}{dx} \quad (5.16)$$

Using this set of equations for the gas and condensed phase and setting them equal to each other yielded input conditions, such as the axial velocity of the fuel, needed for the inputs to the OppDiff code. Solutions for each phase were determined independently and then linked together, where the OppDiff code (used in CHEMKIN) solved the gas-phase equations while the Octave code solved the condensed phase equations.

The gas-phase and condensed-phase solutions were coupled together as mentioned previously by matching the gas velocity at the interface. This was done through an iterative loop in Octave. Figure 5.4 shows a flow chart of the iterative process coupling the Octave code with CHEMKIN's gas-phase solver, implemented through the code provided in Appendix F. The initial estimate for the velocity of the fuel was determined from experimental burning rates found using the PCBE (section 4.1). This burning rate was then used to determine the velocity of the gases leaving the fuel surface. Using conservation of mass, the velocity of the gaseous species pyrolyzing off of the HTPB surface was calculated. This calculated gaseous velocity and

assumed fixed surface temperature of HTPB were used as input conditions for the gas-phase solver, OppDiff.

After CHEMKIN's OppDiff had run through the gas-phase calculations, a heat flux to the surface in Octave was calculated from the gas-phase temperature gradient and the thermal conductivity of the gas mixture at the inlet to the gas-phase CV. This calculated heat flux then was used to re-calculate the burning rate using the condensed-phase code in Octave. Given the new burning rate, a corresponding velocity could be calculated. If the new regression rate differed from the previous value determined from the gas-phase code, a regression rate for the next iteration was obtained based on the difference between the two. This regression rate was then updated to a new velocity, which was used to update the input conditions for the next run of the OppDiff program until a tolerance level was reached. The tolerance specified for the difference in burning rates was set to $1\text{E-}7$ with a scaling factor, a multiplier on the error when determining how much to modify the burn rate for the next iteration, of 0.02 .

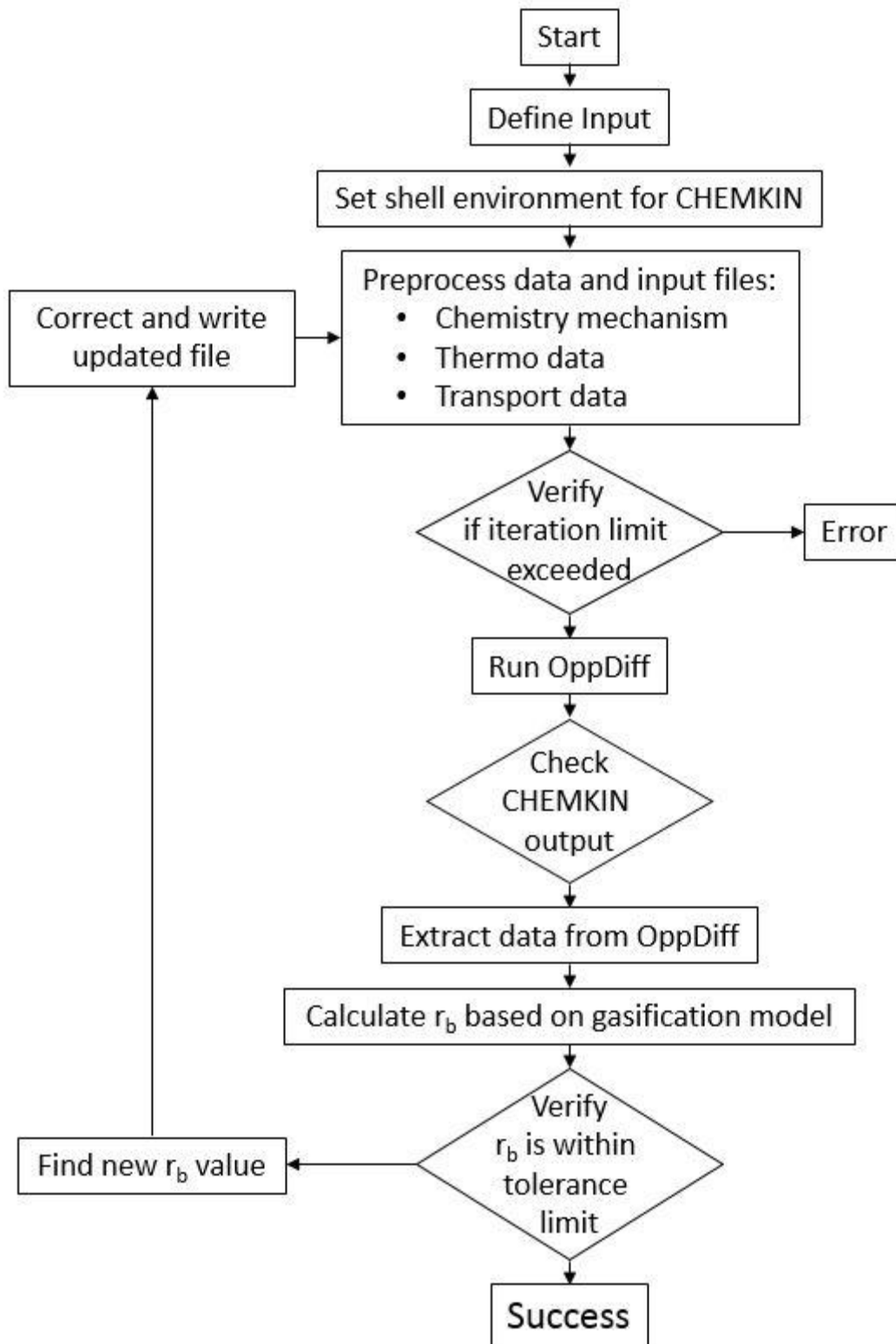


Figure 5.4: Flow chart of coupling in CHEMKIN with Octave.

5.2 Model Inputs

As shown in the flow diagram, input data are needed both for the gas- and condensed-phase codes. For the gas-phase case using CHEMKIN's OppDiff program, a chemical kinetics mechanism, and thermal and transport properties of all the species were required to initiate the gas-phase solver. While the gas-phase inputs are based on known literature reactions and species data, the condensed-phase solver utilized an overall reaction coupled with empirical correlations.

5.2.1 Gas-Phase Model Inputs

The primary inputs required by CHEMKIN's OppDiff code were the detailed chemical kinetics mechanism as well as the transport and thermal properties. The chemical mechanism that was considered was from Glarborg's kinetic mechanism involving hydrocarbon oxidation and hydrocarbon/nitrogen interactions that simulate Natural Gas Reburning. This mechanism was chosen because it included interactions between hydrocarbon oxidation species and nitrogen containing species (including N_2O). The mechanism was initially developed for understanding and characterizing natural gas re-burn technologies as well as NO_x emission control strategies [44].

From Table 5.1, the product species produced by pyrolyzing HTPB were ethene and acetylene. The choice of ethene and acetylene as the decomposition products kept the size of the mechanism to one that permitted parametric studies minimizing computational time.

As for the thermal and transport properties, CHEMKIN's included files from GRI-Mech 3.0 were used; although there were some missing properties which had to be added; the resulting modified thermal and transport data are provided in Appendix G.

5.2.2 Condensed-Phase Model Inputs

The only condensed-phase species is HTPB and the condensed-phase model considered HTPB pyrolysis at the fuel surface producing gaseous products. The properties necessary to determine the heat feedback from the flame to the control volume were density and specific heat, as well as the heat of pyrolysis to calculate the velocity of the gases coming off the surface of the solid fuel (out of the control volume).

The density of the pyrolysis product gases as a function of temperature was calculated using the ideal gas law. It was assumed that ethene and acetylene would behave as ideal gases since the critical conditions of ethene are: 282.35 K and 5.04 MPa [45] and the critical conditions of acetylene are: 308.9 K and 6.138 MPa [46]. The temperatures observed in this study are higher than the pyrolysis of HTPB at 500 K; well above the critical temperature, but below the critical pressure. The ideal gas equation is given by Eq. 5.17.

$$P = \rho RT \quad (5.17)$$

The specific heat as a function of temperature was required to account for the specific enthalpy change through the control volume. This specific heat value was obtained from the DIPPR (Design Institute for Physical Properties) database for C_2H_4 . The empirical correlation was a second-order polynomial valid over a wide range of temperatures ($60 < T < 1500K$). The correlation used is shown below in Eq. 5.18.

$$Cp = A + B * \frac{\frac{C}{T}}{\sinh\left(\frac{C}{T}\right)} + D * \frac{\frac{E}{T}}{\cosh\left(\frac{E}{T}\right)} \quad (5.18)$$

The coefficients are provided in Table 5.2.

Table 5.2: Coefficients from DIPPR for specific heat [47]

A	B	C	D	E
3.3338E4	9.479E4	1.596E3	5.51E4	7.408E2

The change in enthalpy was obtained from Eq. 5.19.

$$\Delta h = \int_{T_1}^{T_2} C_p dT \quad (5.19)$$

The equation of C_p was integrated as an indefinite integral to obtain the change in enthalpy with the temperatures substituted after the gas-phase analysis in CHEMKIN.

To determine the thermal conductivity into the control volume, the mixture thermal conductivity was taken from CHEMKIN. This mixture thermal conductivity was then averaged between the two nearest grid point temperatures to get the most accurate value for the thermal conductivity.

5.2.3 Initialization and Inputs

Regression rate data from the counterflow burner worked well as an initial guess for the velocity of the fuel (ethene and acetylene). Using conservation of mass, the velocity of the gas evolving from the pyrolyzing surface could be determined. This velocity was then used as an initial guess input to the gas phase solver. HTPB pyrolyzes over a range of temperatures. The initial surface fuel temperature of 590 K was chosen due to an empirical correlation utilized for the thermal conductivity for ethene that was bound to a maximum temperature of 590 K. This temperature was set as the initial inlet temperature of the C_2H_4/C_2H_2 gas leaving the surface, while ambient temperature (298 K) was chosen as the inlet temperature of the oxidizer. To make certain a fixed inlet temperature of the fuel was an appropriate boundary condition, the temperature of the surface was varied and the sensitivity of the regression rate was determined

for this variation. The solid fuel pyrolysis law that relates regression rate to the surface temperature is through an Arrhenius equation as shown below:

$$\rho_f r = A \exp^{\frac{-E_a}{2R_u T}} \quad (5.20)$$

where E_a is the activation energy (11.5 kcal/mole), A is the pre-exponential constant (1.59 g/cm²s), and R_u is the universal gas constant. These values for the Arrhenius rate equation were determined from HTPB high heating rate pyrolysis data for a surface temperature range of 500 K to 1000 K [36]. A change in surface temperature from 520 to 547 K results in a change of regression rate on the order of 5%, showing that the assumption of a constant temperature is reasonable.

The initial grid was 100 points, but refined when proven necessary, in the event there was no convergence. Curvature and gradient limits were set to 0.25 and 0.09, respectively. These values were changed based upon the location of the flame, with a grid being setup for each pressure based on the grid structure from the previous solution, producing a refined grid near the position where the flame relocated with the change in pressure. Once a solution was found, the grid was refined to assess and make sure the solution did not change, providing confidence in the results.

CHAPTER 6: Theoretical Results and Discussion

From the experimental results a pressure dependence was observed for N_2O and HTPB in the PCBE. The model described in Chapter 5, was developed to study the N_2O and HTPB flame structure at many different pressure conditions ranging from atmospheric to 1.827 MPa (250 psi). The predicted burning rates were compared with those measured over this pressure range and the analysis of the flame structure is used to better understand the combustion process.

6.1 Burning Rate

Predicted burning rates for the HTPB fuel with N_2O were calculated over the range of 0.101 MPa to 1.827 MPa. Comparison of the calculated and measured linear regression rates are shown in Figure 6.1. Agreement between the calculated rates and experimental data is within a factor of two, with the overall trend being the same.

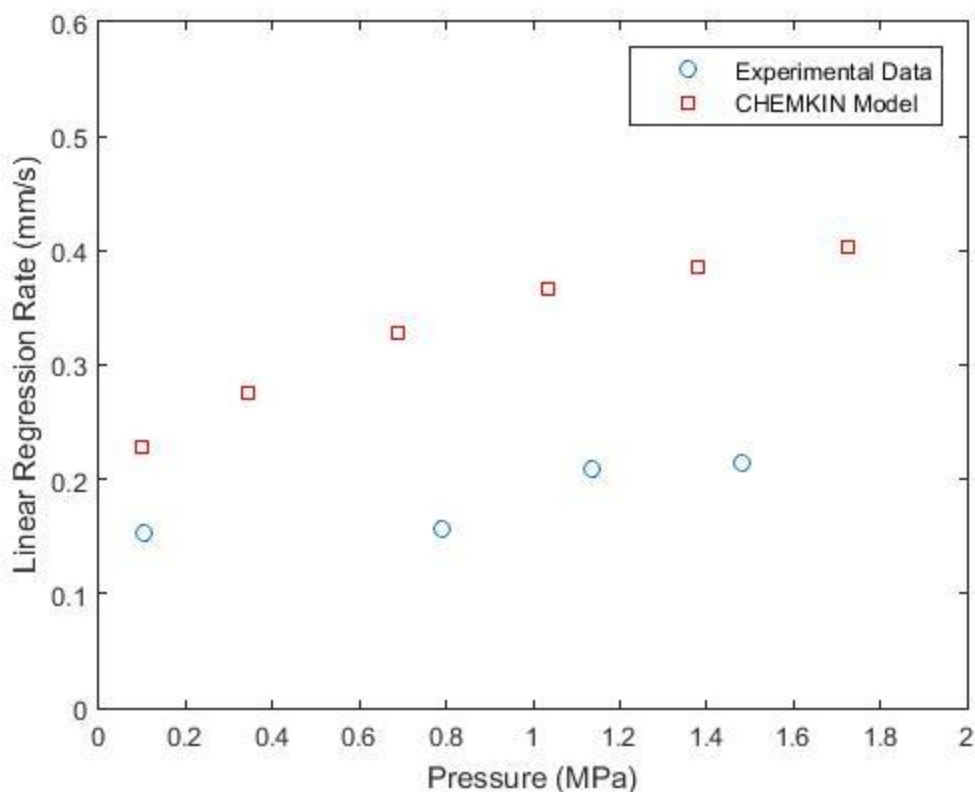


Figure 6.1: HTPB linear regression rate as a function of pressure for both experimental combustion experiments as well as CHEMKIN model results with N_2O .

The same trend is observed with increasing pressure for both the experimental and modeling results using N_2O . The regression rate is observed to increase with pressure and asymptotes to a nearly constant value. Burning rates for the experimental results were lower than the calculated values. This is believed to be due to uncertainties in the condensed-phase mechanism as well as heat loss through the pellet holder in the counterflow burner, which is not considered by the numerical model. Ethene and acetylene were the only fuels included in the mechanism, while Table 5.1 displays the amount of different gases evolving from the pyrolyzing HTPB surface. Figure 6.2 displays the CHEMKIN modeling linear regression rates for both N_2O and O_2 . The model shows that with increasing pressure there is an increase in regression rate,

with oxygen reaching regression rates higher in magnitude than the N_2O , which was observed in experimental testing as well. As will be shown later, the higher regression achieved with O_2 is due to the N_2 diluent produced by decomposing N_2O reducing the maximum flame temperature and temperature gradient at the surface, resulting in a lower linear regression rate. Lehman *et al.* performed both a computational and experimental study on non-premixed combustion of ethene, methane, and O_2 with mixed percentages of N_2 and N_2O , observing extinction limits. It was found that the addition of N_2O into the oxidizer stream decreased the extinction strain rate. Therefore, the flame was inhibited by the addition of N_2O [48]. The cause of N_2O inhibiting the reactions within the flame could be another reason for the reduced regression rates with N_2O .

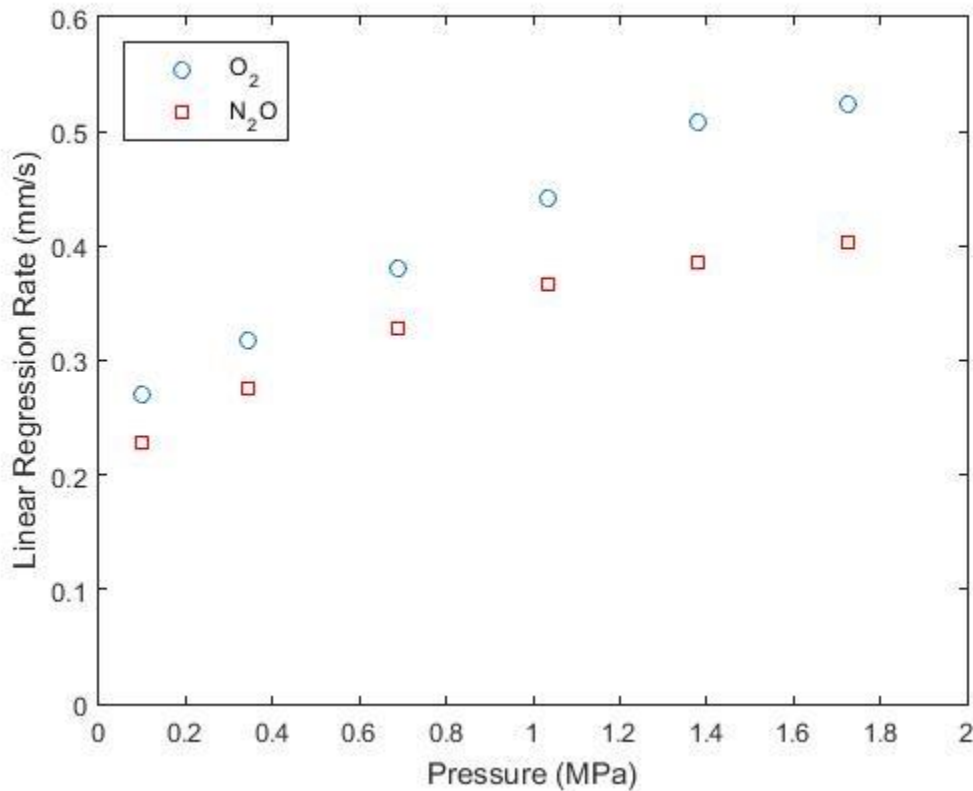


Figure 6.2: HTPB linear regression rate as a function of pressure calculated using the CHEMKIN/Octave model for N_2O and O_2 .

Since the fuel input temperature was chosen as a fixed condition, the regression rates obtained from the model were used to calculate the corresponding temperature with an Arrhenius expression. The temperature decreased to 540K from 590K depending on the regression rates shown in Figure 6.1 (which was discussed in section 5.2.3). This temperature was then input into the CHEMKIN gas solver to determine what percentage the regression rate would change. The regression rate percentage difference for all pressures was under 3% showing that a fixed fuel inlet temperature was a valid assumption.

6.2 N₂O and HTPB Flame structure

By doing an analysis of the species and temperature in the N₂O and C₂H₄/C₂H₂ flame, a better understanding of the overall flame structure and regression rate can be reached. To understand the most fundamental behavior with the C₂H₄/C₂H₂ and N₂O reaction, equilibrium values were calculated in CHEMKIN. Equilibrium flame temperature and species concentrations were found over the pressure range of interest and are shown in Figure 6.3.

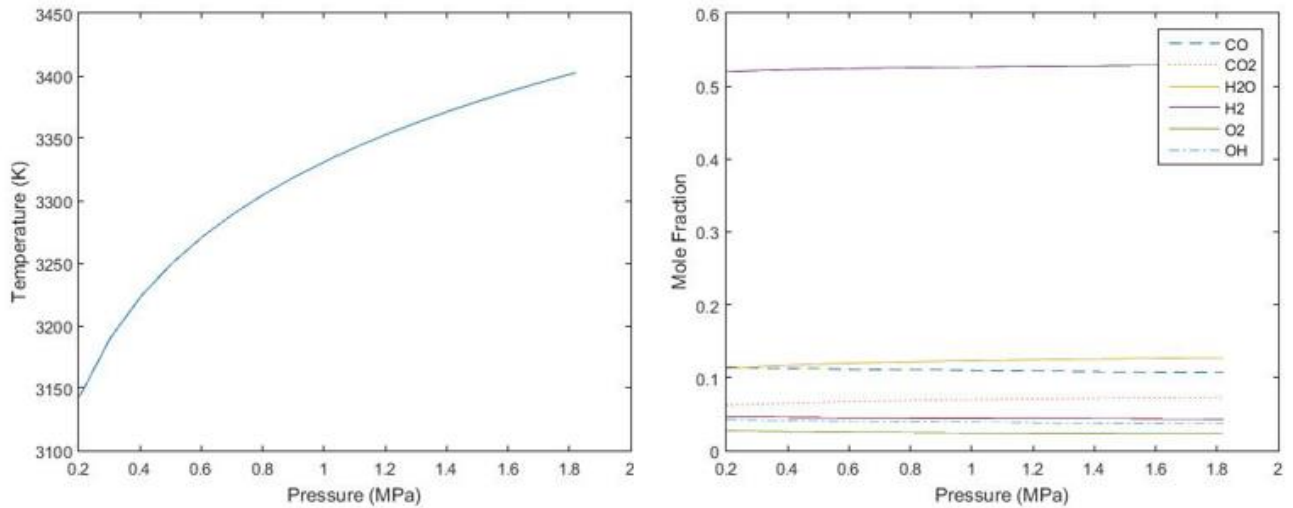


Figure 6.3: Equilibrium mole fractions and temperature as a function of pressure for the C₂H₄/C₂H₂-N₂O flame.

Temperature increased approximately 359K, from 3122.7 to 3482.2K, approximately a 11% increase. With an increase in pressure and a corresponding increase in flame temperature, the major species of (CO_2 and H_2O) are also observed to increase by approximately 20%, with the minor species, such as CO and H_2 and OH , decreasing. As the pressure increases, less dissociation occurs, and therefore the adiabatic flame temperature is shown to increase [23]. Understanding the chemical equilibrium allows for a foundation of the driving force for chemical kinetics. In diffusion flames, the fuel and oxidizer diffuse toward each other at rates that are in stoichiometric proportion. Independent of overall mixture strength, since fuel and oxidizer diffuse together in stoichiometric proportions, the flame temperature approaches the adiabatic flame temperature [49]. The increase in temperature with pressure is also consistent with the increase in regression rate with pressure.

Detailed species and temperature profiles for the $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ and N_2O flame were obtained as part of the gas-phase solution from CHEMKIN's OppDiff when the burning rate was determined. Calculated results of temperature, heat release, and species profiles, from 0.101 MPa and 1.827 MPa are shown in Figure 6.4 and Figure 6.7, respectively. The trends that occur in both plots are fairly similar, with the reactions occurring over a shorter distance, decreasing the flame thickness, at the higher pressures, as well as moving the flame's location closer to the fuel surface (on the plot axis, 0 mm=fuel side, 5 mm=oxidizer side).

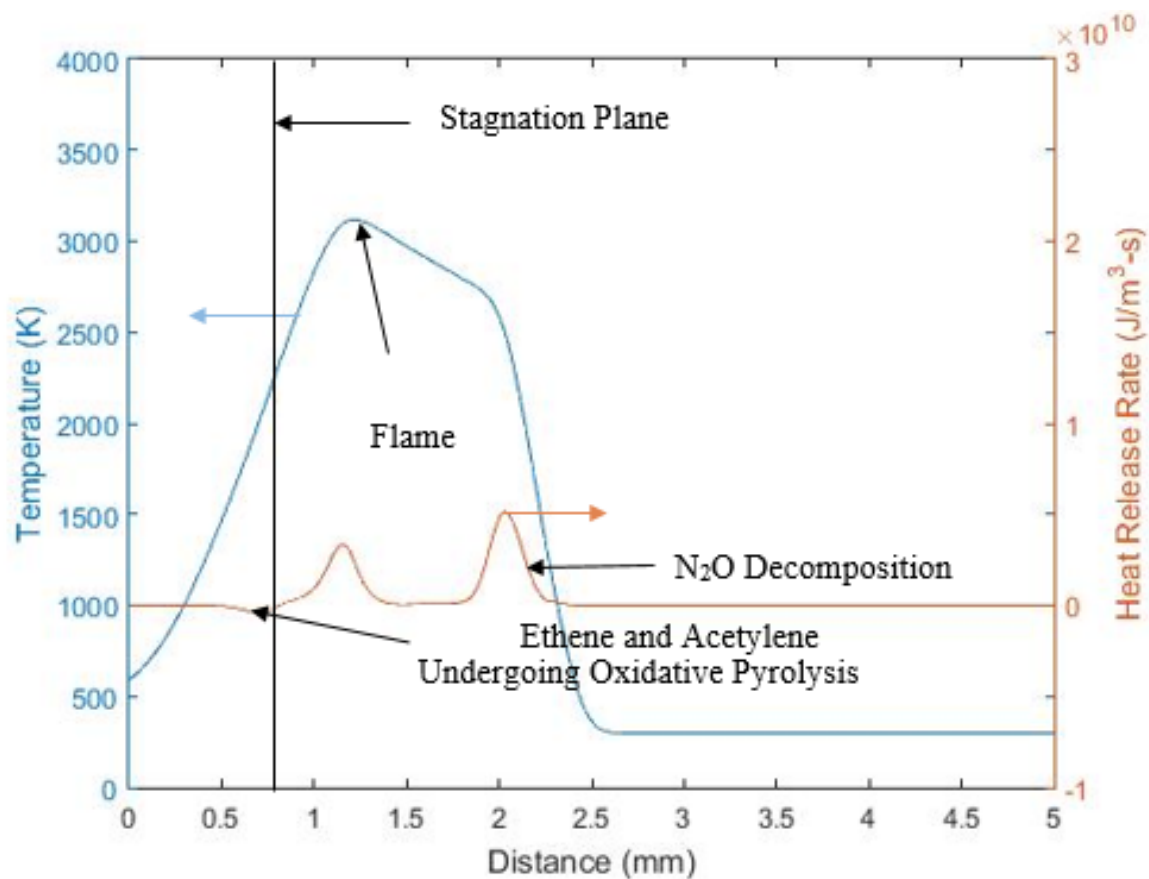


Figure 6.4: Calculated temperature and heat release rate for a $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame at atmospheric pressure. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner. The point of highest temperature sits in the near-fuel surface region on the oxidizer side of the stagnation plane.

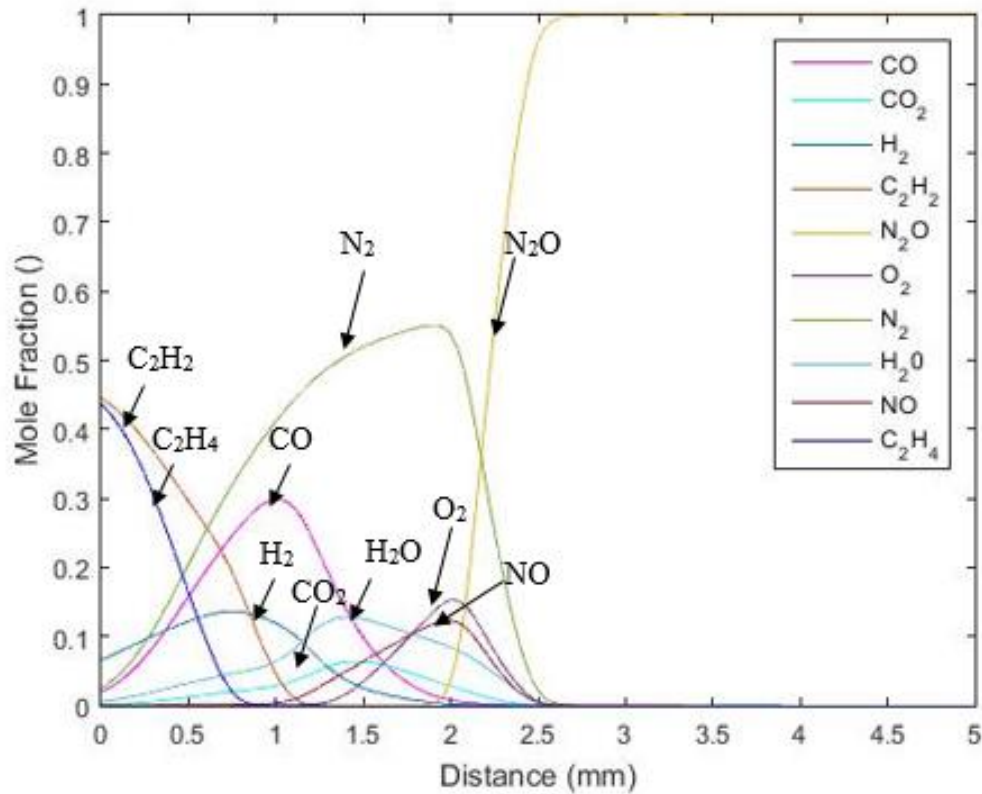


Figure 6.5: Calculated species profiles for a $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame at atmospheric pressure. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

For the 0.101 MPa case, the flame temperature increased to a temperature of 3115 K close to the equilibrium value. In the limit of infinite kinetics a diffusion flame is confined to a thin reaction sheet. When finite rate kinetics are considered, complete combustion does not occur, allowing the products and reactants to diffuse through the reaction zone causing a slightly lower temperature than the equilibrium value.

Major species included the fuel (C_2H_4 and C_2H_2), product species such as H_2 , H_2O , CO , CO_2 , and N_2 , and the oxidizer N_2O . The peak product species N_2 , H_2O , and CO_2 were close to

the equilibrium values. The higher CO concentration relative to CO₂ was observed from both the equilibrium, and diffusion solver. This increase in CO is produced by the CO₂ dissociation (which dissociates at 3100K) [50]. Figure 6.4 indicates that there are three distinct zones, one endothermic zone and two exothermic zones. One exothermic zone is associated with the N₂O decomposition to N₂ and O₂ while the second is the oxidation process. The endothermic event is associated with the ethene and acetylene undergoing oxidative pyrolysis, which will be discussed later. To get a better understanding of the regression rate dependence with increasing pressure the flame structure at a higher pressure was also considered.

At 1.827 MPa, the temperature gradient at the fuel surface is observed to increase, with the overall flame thickness decreasing. The peak flame temperature is 3363 K, which is close to the equilibrium value and higher than that of the atmospheric case. With an increasing pressure, the overall reaction rate increases, decreasing the flame thickness and increasing the temperature. Along with the reduction in the size of the flame thickness, the flame's location is also shown to shift closer to the fuel side. The increase in regression rate and shift in flame location is contradictory to the expected behavior of an ideal diffusion flame, where the effects of pressure should be negligible. This change in the flame's location will be discussed later. The two distinct exothermic zones have changed under higher pressure conditions as shown in Figure 6.6. The exothermic peak for N₂O decomposition still exists, however, the exothermic peak associated with the oxidation reaction is now distributed over a wider spatial domain containing many reaction zones with larger exothermicities. In Figure 6.7 the O₂/NO ratio is much larger at the higher pressure and there is no leakage of O₂ and NO into the fuel pyrolysis zone indicating faster reaction rates. The overall species fractions of H₂, H₂O, CO, CO₂ and N₂ were nearly identical to that of the atmospheric case.

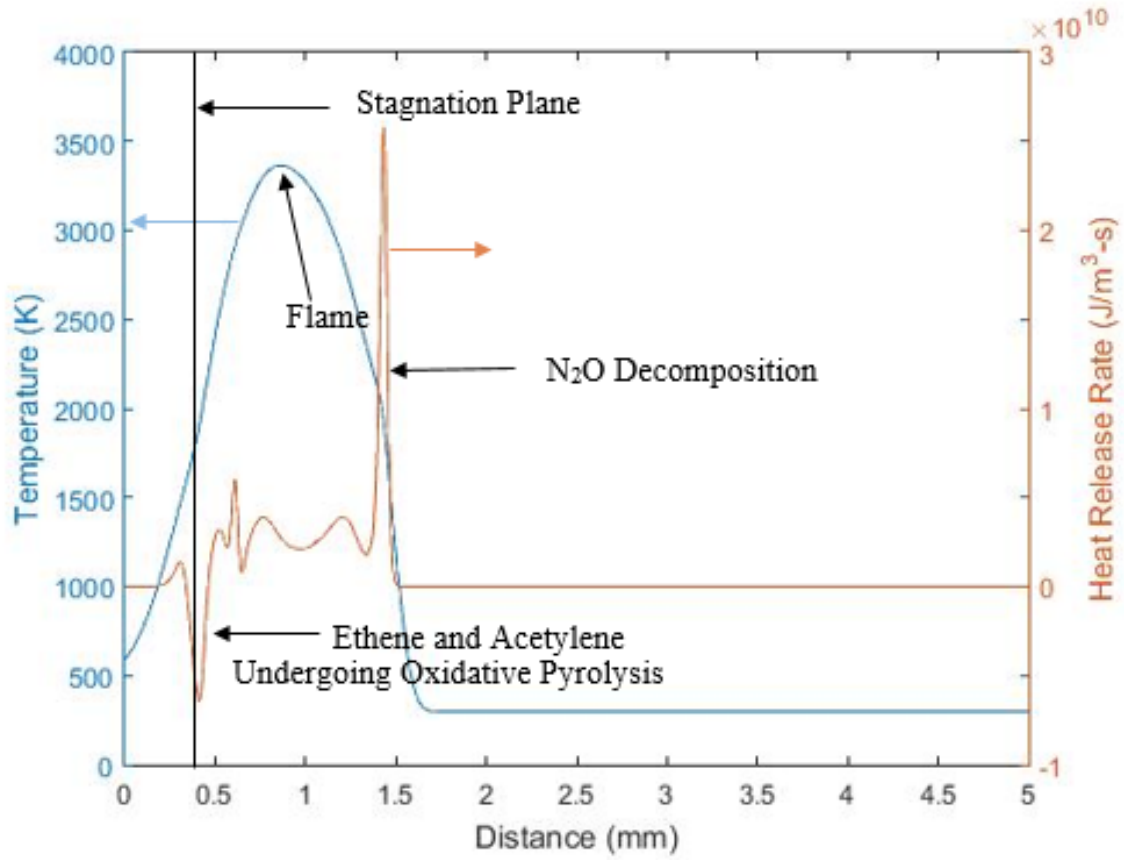


Figure 6.6: Calculated temperature and heat release rate for a $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame at 1.827 MPa. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner. The point of highest temperature sits in the near-fuel surface region on the oxidizer side of the stagnation plane.

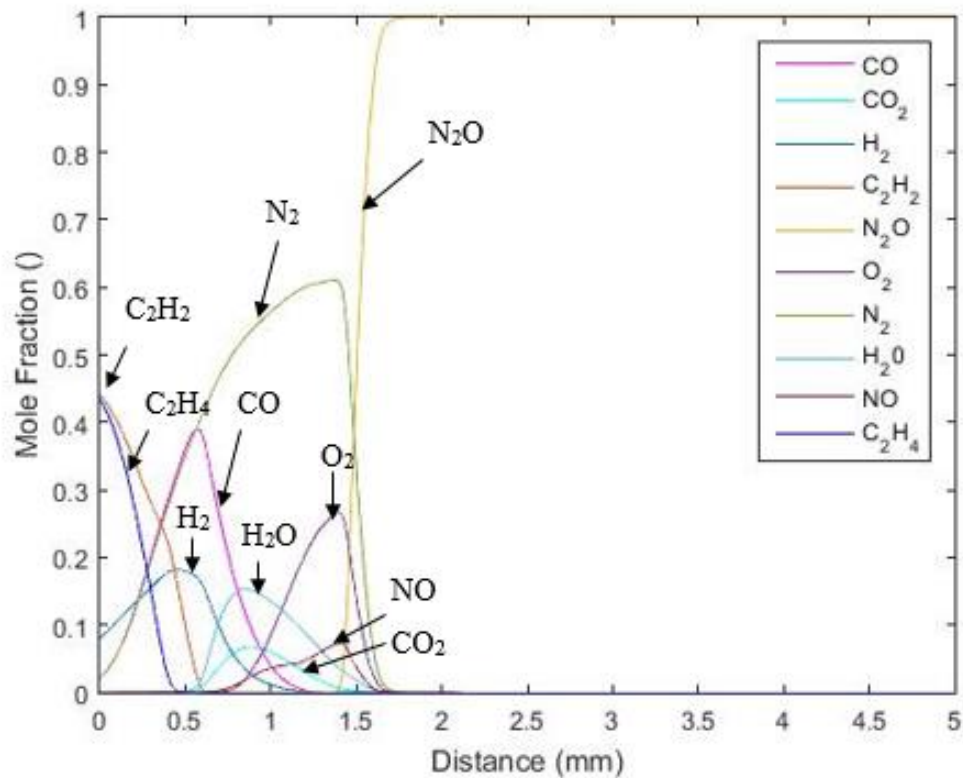


Figure 6.7: Calculated species profiles for a C_2H_4/C_2H_2 N_2O flame at 1.827 MPa. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

Although no distinct stages are observed in the temperature profile, examination of the heat release rate (HRR) and species profiles shows regions and reactions based on the chemical composition trends. The description given here is based upon the atmospheric case (Figure 6.4), as the 1.827 MPa case shows similar trends, except the decrease in flame thickness and the movement of the flame closer to the solid fuel surface. This is shown in better detail in Figure 6.8, where it is evident that the flame is becoming confined to a thinner region as pressure is increased. The flame is also shown to shift toward the fuel side with increasing pressure. Specific effects of the pressure in the structure will be discussed later.

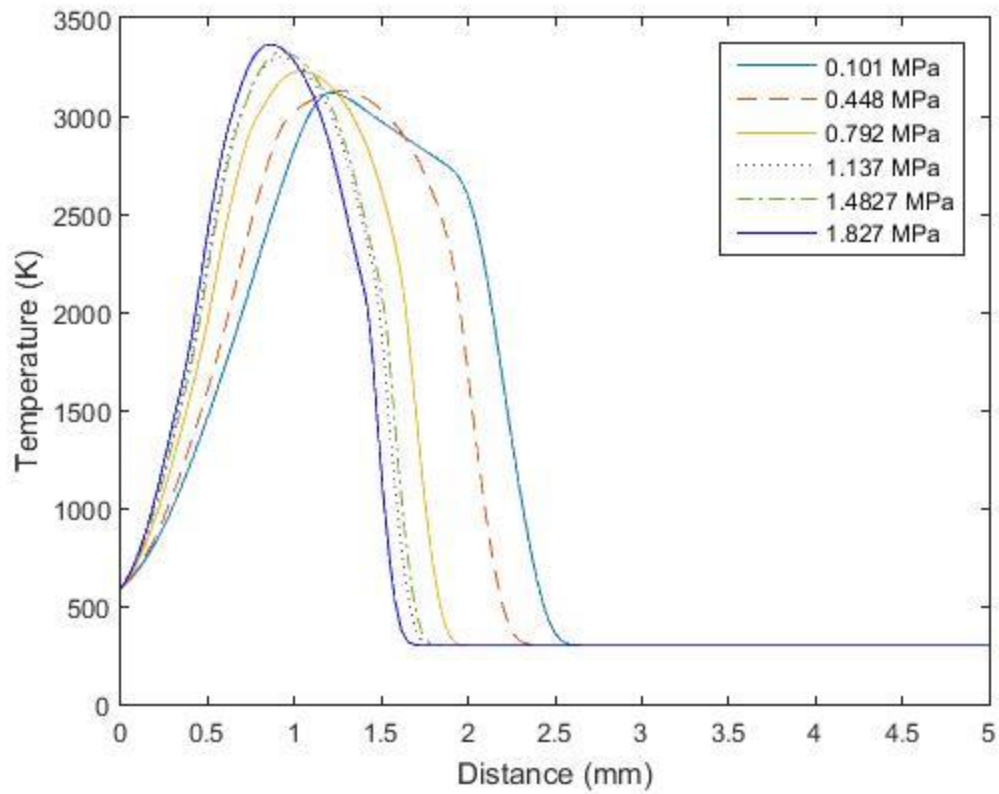


Figure 6.8: Calculated temperature for a C_2H_4/C_2H_2 N_2O flame at the given range of pressures. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

A diffusion flame's stagnation plane sits at the region where the momentum fluxes, between the oxidizer and fuel streams, are equal, and where the velocities go to zero as mentioned in section 2.1, this can be observed in Figure 6.9.

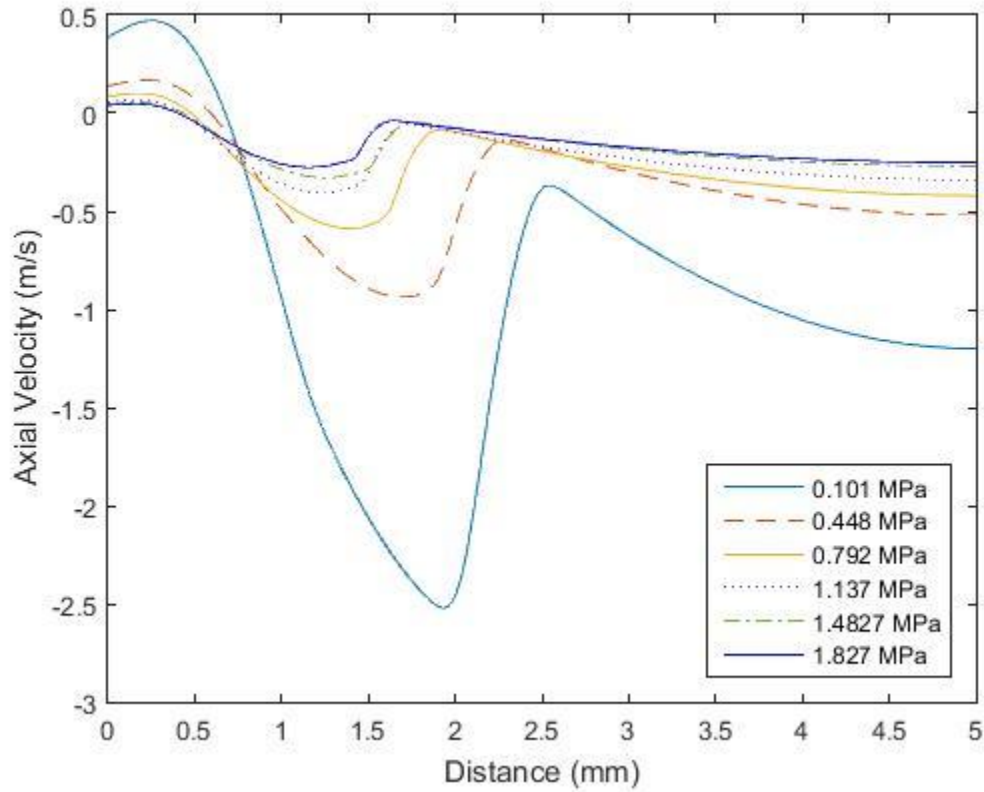


Figure 6.9: Axial velocity of the C_2H_2/C_2H_4 N_2O flame at the given range of pressures. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

The velocity goes to zero at 0.7mm, while the flame is located at 1.12mm at atmospheric pressure. This shows that the flame sits on the oxidizer side of the stagnation plane. Figure 6.9 also displays that the stagnation plane and, therefore flame moves closer to the fuel surface with increasing pressure. Even though the mass regression rate is shown to increase with increasing pressure, the blowing velocity of the pyrolysis products evolving from the fuel surface decreases

with pressure. As shown in Eq. 5.2 the velocity and density are linear. Between 0.101 MPa and 0.448 MPa the density magnitude triples while the velocity magnitude decreases by a factor of two. Therefore, the mass regression rate is going to increase, but the momentum flux will decrease. Both the momentum flux and velocity of the gas (C_2H_4/C_2H_2) as well as the constant momentum flux of N_2O , can be seen in Figure 6.10.

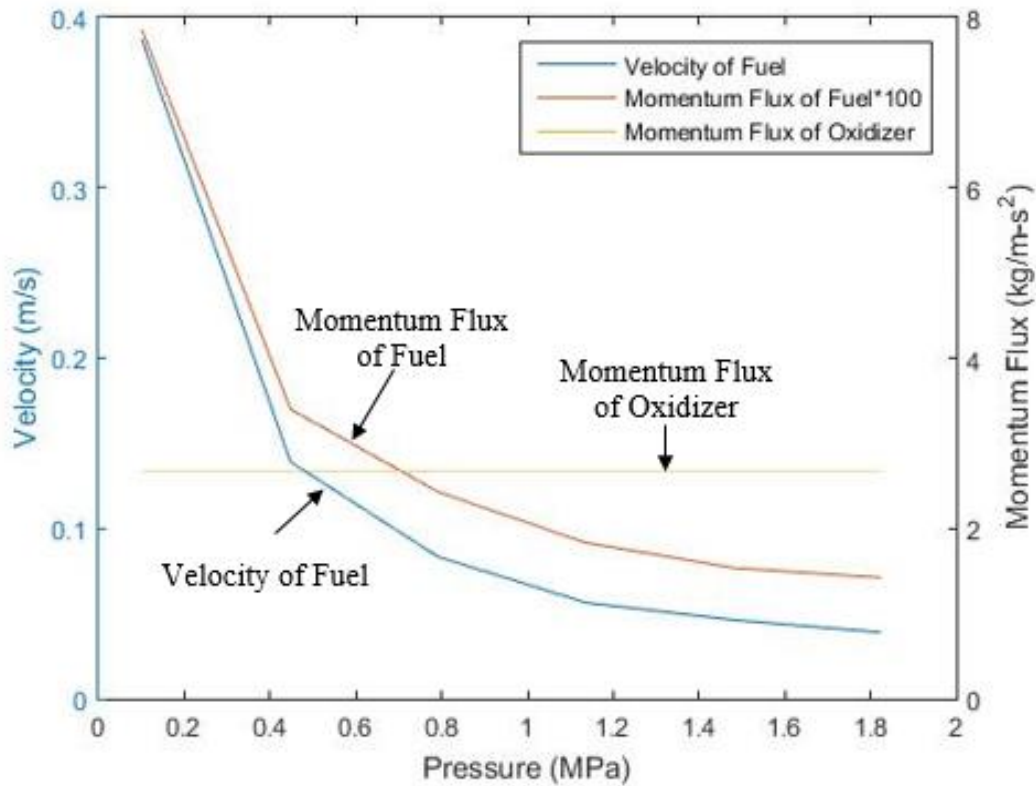


Figure 6.10: Velocity and momentum flux of the gaseous fuel and momentum flux of N_2O as a function of pressure.

In the momentum equation, the velocity is a squared function, while the density is linear as shown in Eq. 4.1. Since the stagnation plane sits in between the spatial domain of the fuel surface and oxidizer tube exit, this will move the flame closer to the fuel surface with increasing

pressure, due to the constant momentum flux of the oxidizer and decreasing momentum flux of the fuel.

The flame's location typically exists at the highest level of heat release (i.e, highest temperature). In the C_2H_4/C_2H_2 N_2O flame this is not the case. As shown in Figure 6.4, the highest heat release rate is at 2.21mm. This is not the position of the flame's location, but rather heat release from N_2O decomposition, which is a highly exothermic event. Utilizing CHEMKIN PRO's reaction path analyzer, the reactions occurring at that particular location can be analyzed. As shown in Figure 6.11 one of the reaction pathways occurring at the highest level of HRR is the decomposition of N_2O , with the highest HRR coming from Reaction (6.1).

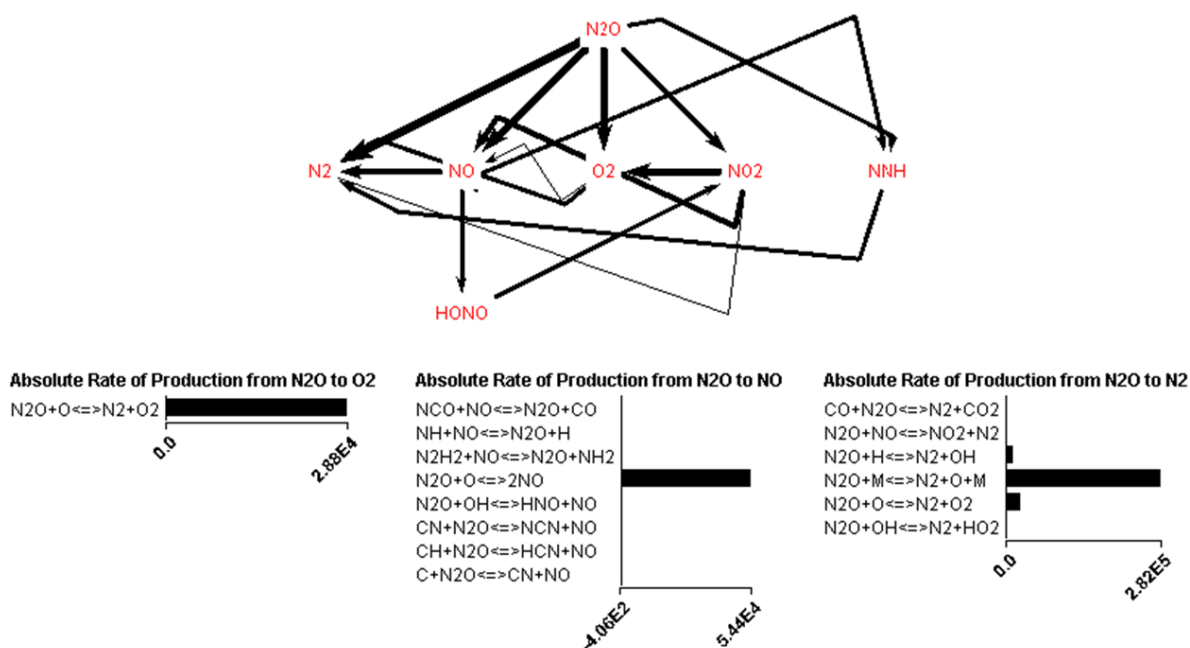


Figure 6.11: Reaction pathway of N_2O decomposition at 2.21 mm.

It is evident from the reaction pathway analysis that the N_2O dissociates to form N_2 , NO , O_2 , and to a lesser degree NNH and NO_2 . The dissociation of the N_2O is what produces the O_2 , and at the maximum level of HRR the mixture fraction of O_2 is at its greatest. This dissociation of the N_2O to form O_2 is what reacts with the CO and H_2 produced from the oxidative pyrolysis of the C_2H_4 and C_2H_2 . Therefore, from that location in the flame, the fuel and its intermediates react as it would with O_2 as the oxidizer. However, given the extra species associated with N_2O , such as N_2 and NO , the resulting flame temperature will be lower than pure oxygen, due to the N_2 diluent [51]. The flame structure then seems to follow that for combustion of a $C_2H_4/C_2H_2 - O_2$ system, as observed in Figure 6.12, showing the HRR and temperature profile for a C_2H_4/C_2H_2 and O_2 diffusion flame at atmospheric pressure. There are still two exothermic regions, however, the second exothermic reaction has a smaller peak and is distributed over a greater spatial region. The reaction corresponding to the largest HRR in the O_2 flame is Reaction (6.2):



The temperature and HRR profiles have the same general trends, but the peak magnitudes of the temperature and HRR are higher for the O_2 flame compared to the N_2O flame. There also exist two small endothermic regions, the first one again associated with the oxidative pyrolysis of the C_2H_4 and C_2H_2 while the second appears to result from the dissociation of CO_2 and H_2O where the flame temperature is the highest.

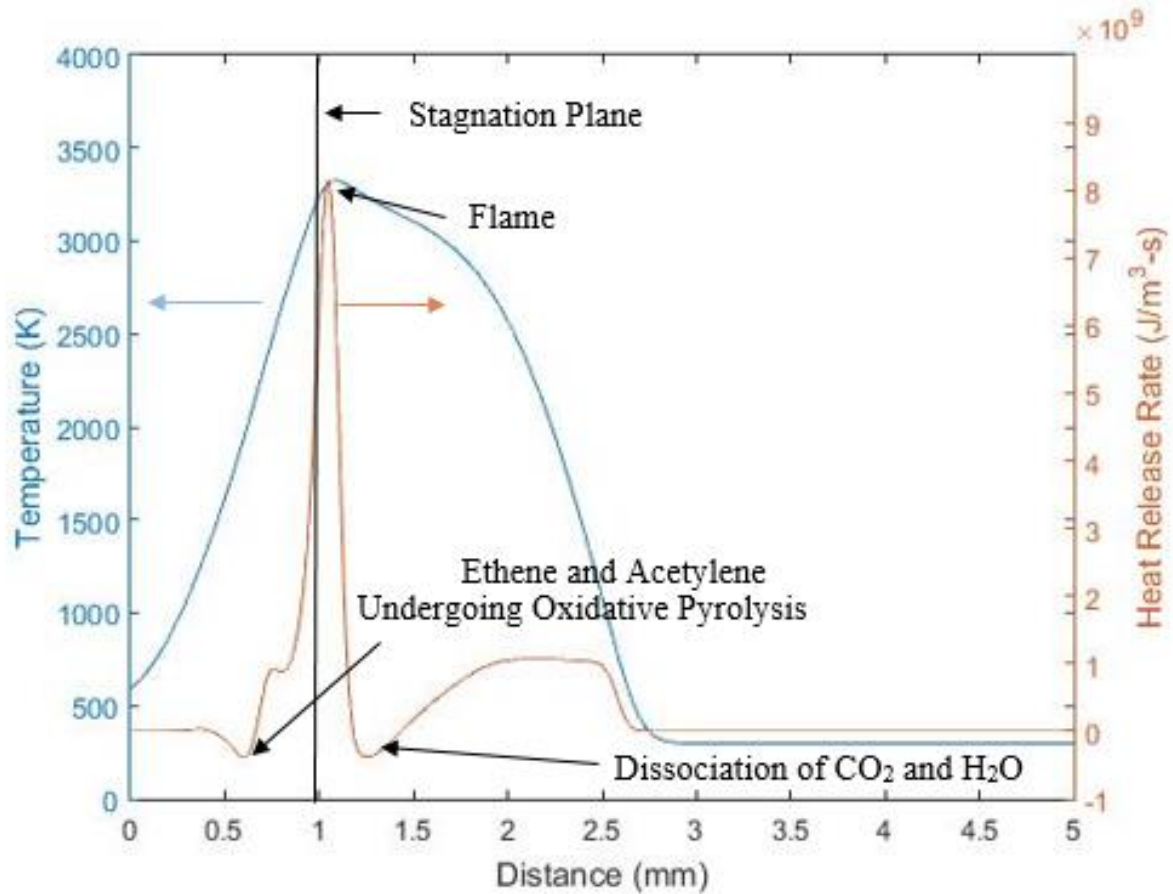


Figure 6.12: Calculated temperature and heat release rate for a $C_2H_4/C_2H_2/O_2$ flame at atmospheric pressure. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner. The point of highest temperature sits in the near-fuel surface region on the oxidizer side of the stagnation plane.

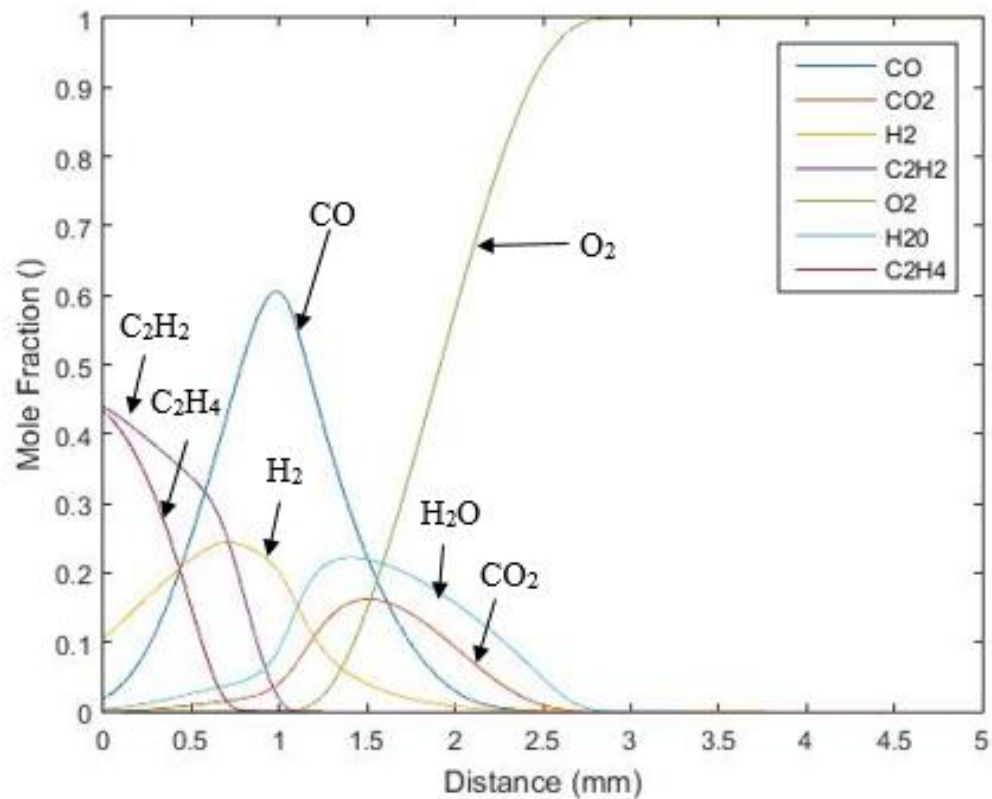


Figure 6.13: Calculated species profiles for a C₂H₄/C₂H₂ O₂ flame at atmospheric pressure. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

Understanding the reaction and chain branching of the C₂H₄-O₂ mechanism will shed light as to the endothermic and exothermic events occurring in the HRR profile. Since the N₂O dissociates to form O₂, which is the oxidant that reacts with the fuel, the oxidation of C₂H₄ was looked at in closer depth with the O₂ flame at atmospheric pressure. For ethene the major initiation steps are





Reaction (6.3) is the fastest however Reaction (6.4) is the chain initiator. The H abstraction plays a major step in producing the vinyl radical (C_2H_3). This is shown in the reaction pathways diagram for the pure oxygen case, where the main reaction for formation of C_2H_3 is Reaction (6.4).

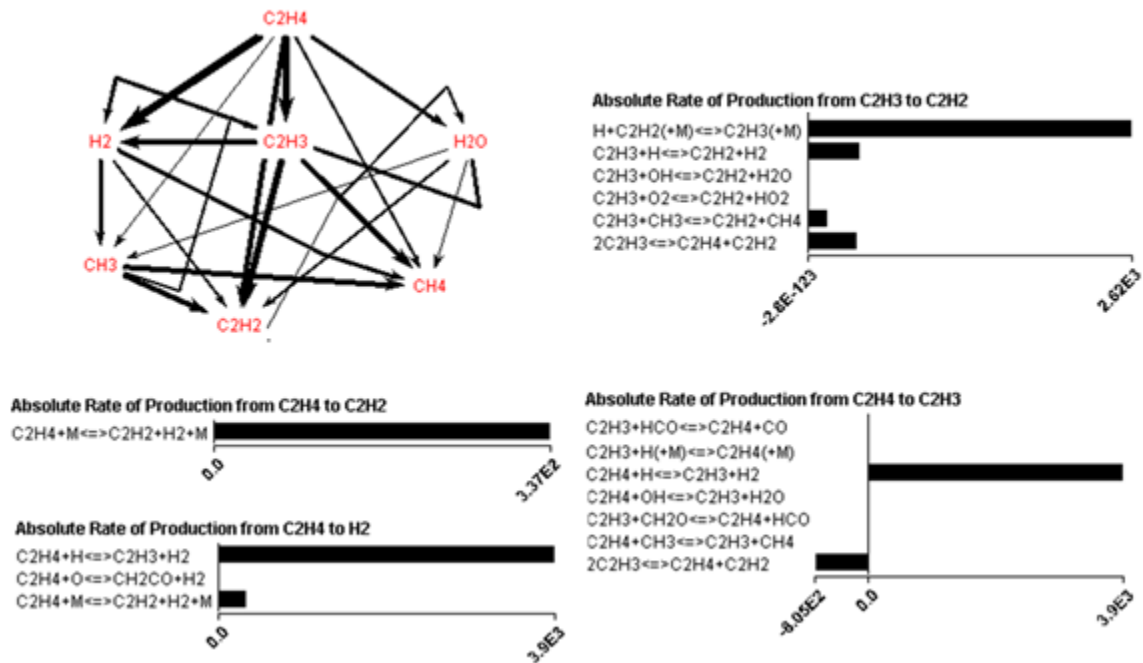


Figure 6.14: Reaction pathway at the endothermic heat release for the O_2 flame at atmospheric pressure located at 0.518 mm.

The majority of the vinyl is consumed by C-H bond scission to form acetylene via:



and to a lesser extent by H-atom radical attack and the bimolecular reaction with itself. Acetylene can be a major product of incomplete fuel rich combustion. This reaction is also shown in the reaction pathway, which is located at the point of endothermic heat release. Reaction (6.5) is the main contributor to this endothermic event, between, 0.5mm and 0.7mm, seen in Figure 6.12.

The reaction between acetylene (C_2H_2) and O is rapid and forms the ketyl radical (HCCO) shown in Figure 6.15 which then proceeds to form the methylene radical (CH_2) as shown in Figure 6.16.

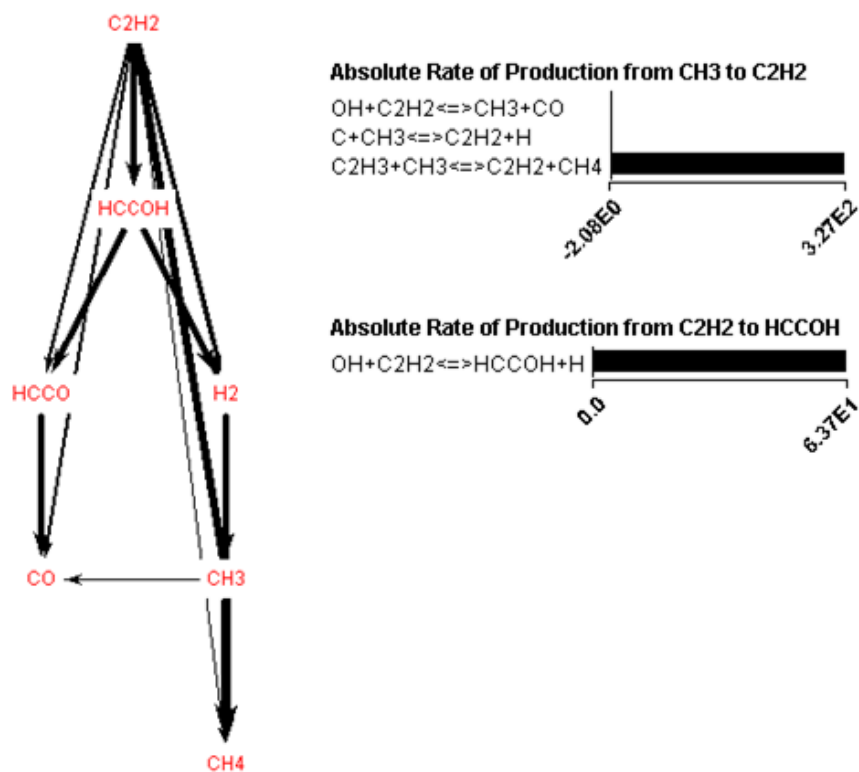


Figure 6.15: Reaction pathway of C_2H_2 near the endothermic event for O_2 at atmospheric pressure.

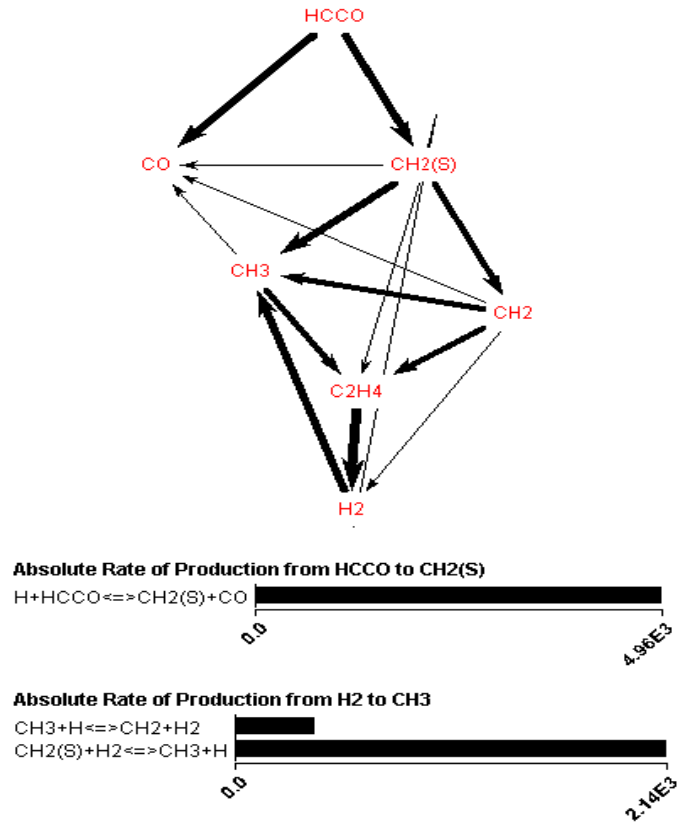


Figure 6.16: Reaction pathway at a location of 0.808mm for HCCO proceeding to the methylene radical for oxidizer O_2 at atmospheric pressure.

Since the mechanism was analyzed in closer detail, the diffusion flame structure must also be examined. Considering the N_2O flame, the stoichiometric mixture fraction is 0.1004, located at 1.46 mm at atmospheric pressure, which is where the flame should sit. Because the location of a diffusion flame is located at the maximum temperature, to understand the location of the flame with respect to mixture fraction, a plot of temperature versus mixture fraction is shown in Figure 6.17. It is clear that the flame at atmospheric pressure is not at stoichiometric conditions. As the pressure increases the maximum temperature moves closer to the stoichiometric mixture fraction, while also shifting slightly closer to the oxidizer side of the

stagnation plane of 0.7mm, 0.429 in mixture fraction space for atmospheric pressure (in CHEMKIN a mixture fraction of zero is the oxidizer, while one corresponds to the fuel).

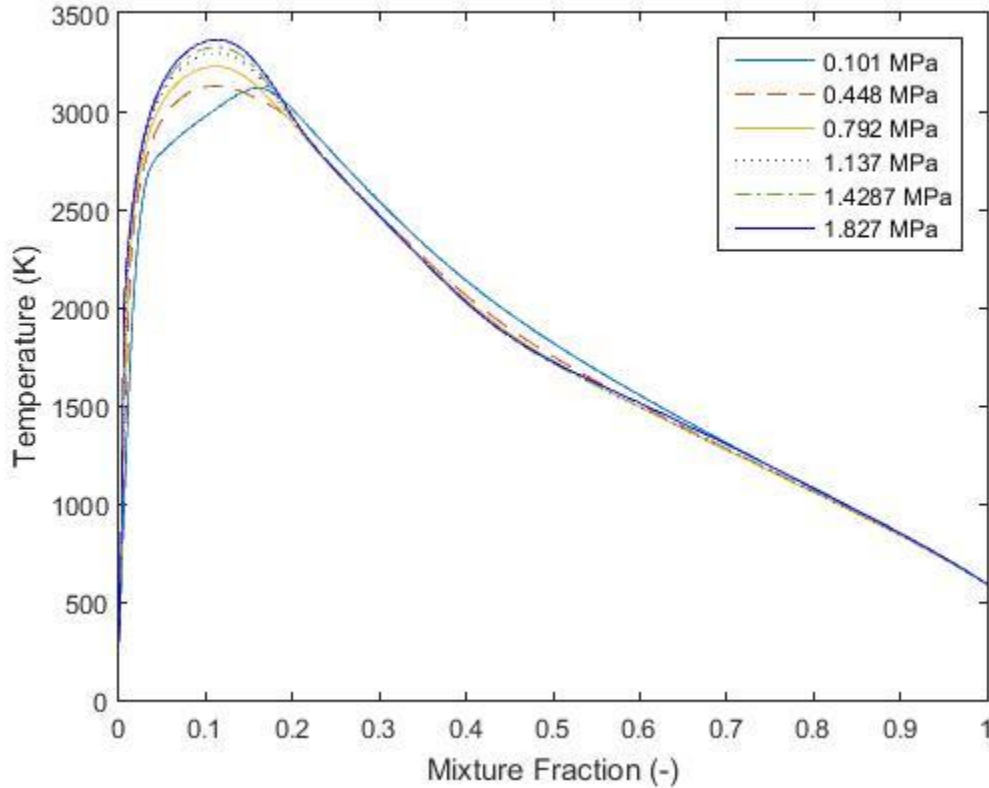


Figure 6.17: Temperature as a function of mixture fraction and increasing pressure for N_2O .

Between 0.101 MPa and 0.448 MPa there is a shift in the maximum temperature, moving closer to the oxidizer side of the stagnation plane. From 0.448 to 0.792 MPa the maximum temperature occurs close to the same mixture fraction. Once the pressure reaches 1.827 MPa it is the closest to stoichiometric conditions.

Also observed with increasing pressure is a decrease in reactant leakage, indicating a closer approximation to reaction-sheet behavior. With increasing pressure and a decrease in reactant leakage, more complete combustion will occur. This is understandable, as the pressure increases the flame shifts towards the stoichiometric mixture fraction, as previously mentioned.

However, the flame is shown to be shifting toward the fuel side as the pressure increases. From simple theory, a diffusion flame's structure should be independent of pressure. Therefore, to see if the flame's location was moving due to the diffusion flame or the surface model coupling implemented by the Octave wrapper, the N_2O case was analyzed at a fixed momentum flux for both the oxidizer and fuel. To obtain data for a fixed momentum case, the fuel and oxidizer velocity was specified in CHEMKIN bypassing the wrapper. Figure 6.18 demonstrates that it is not the diffusion flame causing the pressure dependence, but rather the physical surface model coupling with experimental parameter inputs.

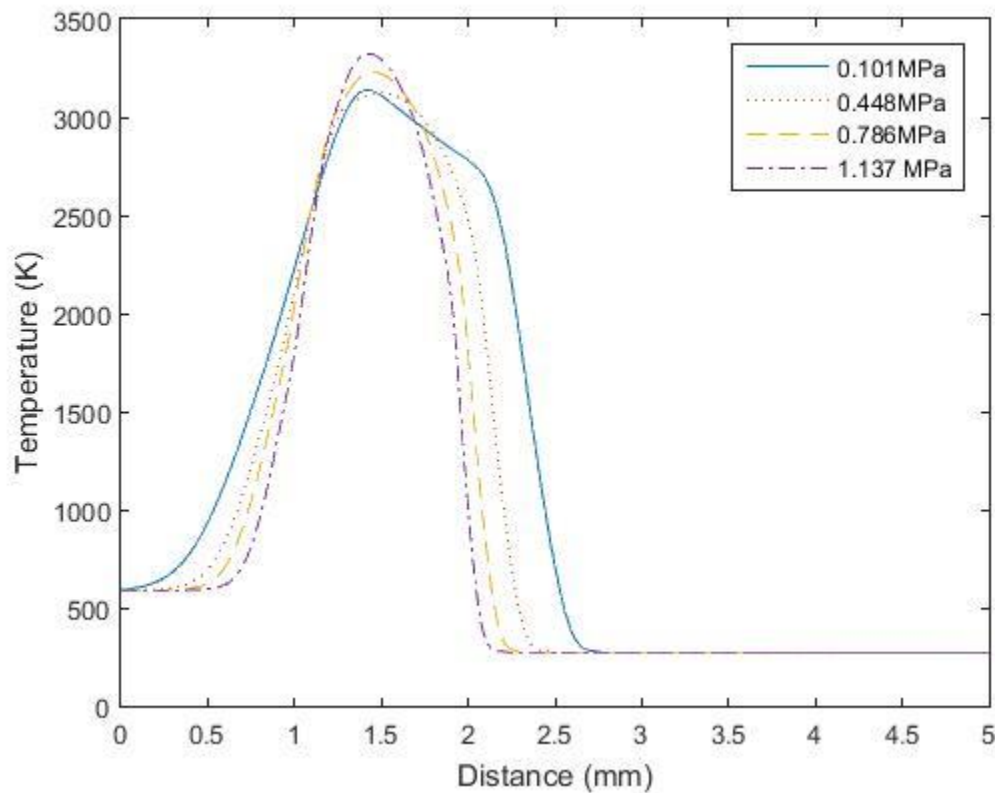


Figure 6.18: OppDiff flame calculation for fixed momentum flux for $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame. The distance corresponds to the separation distance between fuel (0mm) and oxidizer (5mm) in the counterflow burner.

The gasification of the fuel is determined by conductive heat feedback from the gas phase, therefore the slope of the temperature profile just above the control surface of the fuel is what controls the burning rate. As the pressure increases, the flame becomes confined to a thinner region with a higher flame temperature creating an increase in slope. Regression is controlled by heat feedback, primarily conduction, at the surface, which by Fourier's Law is proportional to the temperature gradient, observed with rising pressures. Therefore, the increase in regression rate due to pressure is through the slope of the temperature gradient at the surface.

The results from the modeling indicate some important observations.

1. There was an increase in linear regression rate with an increase in pressure for C_2H_4/C_2H_2 N_2O and O_2 flame. The increase in regression rate with increasing pressure is due to the slope of the temperature gradient and the increasing heat feedback to the solid fuel surface.
2. The flame was observed to become thinner with less leakage of NO and O_2 indicating faster reactions as pressure was increased.
3. The stagnation plane moved closer to the fuel side from the changing fuel momentum flux relative to the constant momentum flux of the oxidizer with increasing pressure. This also attributed to the larger gradient increasing heat feedback at the fuel surface, enhancing the regression rate.
4. The flame structure of N_2O exhibits the same trends as O_2 following decomposition. While the heat release from N_2O decomposition and pyrolyzed fuel oxidation occurs in two distinct regions under atmospheric conditions, but as higher pressures are reached the exothermic heat release due to oxidation becomes distributed over a wider spatial domain reaching larger exothermicities.

5. GOx was observed to have lower regression rates than N_2O , due to the N_2 diluent.

CHAPTER 7: Summary and Conclusions

Counterflow burner and static fired rocket motor experiments were conducted to investigate HTPB and aluminized HTPB solid fuels with the oxidizers N_2O and GOx at pressures ranging from 0.101 MPa to 1.827 MPa. A detailed model using CHEMKIN and Octave was developed to understand the flame structure and pressure dependence observed in the PCBE with N_2O . Aluminized fuel compositions were studied as well to observe any effect of the metallic additives on solid fuel regression rates when combusted with N_2O . Rocket motor experiments were conducted to investigate propulsive performance of such fuels with N_2O as the oxidizer.

PCBE experiments were conducted with HTPB and N_2O , from 0.101 MPa to 1.87 MPa and a pressure dependence on the linear regression rate was observed. The linear regression rate increased from 0.152 to 0.21 mm/s over a pressure range of 0.101 MPa to 1.1 MPa where it then plateaued to a relatively constant value. Although the N_2O decomposition process is pressure dependent, the observed pressure dependence was found mainly to be due to heat transfer to the pyrolyzing surface from the reaction of O_2 with the fuel components, versus N_2O reaction with the fuel components. As the pressure increased, the flame shifted toward the molten fuel surface increasing heat feedback, resulting in an increased rate of solid fuel pyrolysis. Although there was an increase in regression rate with higher pressures, the velocity of the gasses coming off of the solid fuel surface decreased, therefore decreasing the momentum of the fuel. The fixed oxidizer momentum and decrease in fuel momentum caused the $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame to move closer to the fuel surface with increasing pressure. The flame structure was also observed to become thinner, due to faster kinetics with increasing pressure. Heat release from N_2O decomposition and pyrolyzed fuel oxidation occurs in two distinct stages under atmospheric conditions, while at elevated pressure (1.827 MPa) the exothermic peak associated with

oxidation becomes distributed over a wide spatial domain containing many reactions with large exothermicities. Following decomposition, the flame structure of N_2O exhibits the same trends as that of O_2 . The model results predicted experimentally measured solid fuel regression rates within a factor of two. Furthermore, the model indicated similar trends with increasing pressure for both the O_2 and N_2O , and predicted a higher regression rate for O_2 as an oxidizer compared to N_2O .

Spectroscopic data obtained from aluminized counterflow burner experiments showed no indication of AlO or Al with N_2O . AlO emission was captured for experiments conducted using GOx . This can be attributed to the lower regression rates observed with N_2O not reaching sufficient velocities to drag the particles from the molten surface to reach the flame and react. The aluminum was not observed to ignite near the fuel surface in either counterflow burner with N_2O , overall showing a decrease in regression rate with the addition of aluminum particles to the HTPB.

Rocket motor firings were conducted using a static-fired rocket motor to determine the effect of the aluminum addition to HTPB fuel grains when combusted with N_2O . Three solid fuel compositions were investigated: pure HTPB and HTPB containing 10 wt% of Valimet H2 and H12 aluminum particles. Over the baseline HTPB, the linear regression rate increased 15% for both aluminized fuel grains. The empirical regression rate correlation was utilized for the HTPB/H12 aluminum grains to determine a pre-exponential factor of 0.5049 compared to pure HTPB values of 0.417 [35]. The combustion efficiency and chamber pressure for each rocket motor experiment were similar with an average combustion efficiency of 96% achieved for the aluminized grains. The aluminum enhanced the solid fuel regression rate in the hybrid rocket motor, but did not show any improvement in regression rate in the counterflow burner. The

higher shear forces across the surface in the motor may also drag the particles along the surface to the post combustion regime. The lack of AlO emission and observed accumulation of aluminum particles in the surface melt in the counterflow burners suggests the velocity of the gaseous pyrolysis products evolving from the fuel surface was insufficient to drag the particles from the viscous surface melt. Slower regression rates would also indicate a thicker melt layer, where more particles could accumulate. Future experiments should be considered employing higher oxidizer velocities to determine whether aluminum particle entrainment can be achieved, and enhanced regression rate result using the counterflow configuration.

7.1 Future Work Recommendations

- 1) Extend the experiments in the PCBE with N_2O to higher pressures and higher oxidizer flow rates. This will shed light onto whether or not the linear regression rate will continue to plateau. By obtaining higher oxidizer velocities this will increase the linear regression rate, in turn increasing the velocity of the gaseous pyrolysis products evolving from the fuel surface, to determine what velocity is needed to entrain the aluminum in the flame.
- 2) To obtain regression rates in the model the surface temperature was held constant. Given the Arrhenius kinetics provided, the regression rate only varied 3% with a 5% change in surface temperature. However, the products from the pyrolysis reaction are known to shift significantly with temperature. Therefore, it would be valuable to modify the condensed phase model to include the change in surface products, with varying surface temperature. The code can be altered to calculate the temperature from the Arrhenius expression for a given regression rate. Given the surface temperature the species evolving from the HTPB surface can be inputted into the model. A micro-thermocouple embedded into the pellet to measure the temperature profile as the surface regresses will allow for a more accurate understanding of the experimental condition to be observed.
- 3) Compare the $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2O flame to a $\text{C}_2\text{H}_4/\text{C}_2\text{H}_2$ N_2/O_2 flame to understand the effect of oxidizer exothermic decomposition, and N_2 dilution on the regression rates and flame structure.
- 4) Modify the condensed phase and gas-phase models to consider metal particles in the solid fuel, this will help understand the effect condensed phase particles have on the

regression rate, through radiation and the added heat of combustion. This can be accomplished using Data Parallel Line Relaxation CFD code (DLPR) to couple the condensed phase particles to the gas-phase model.

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Appendix A: Sample of NASA CEA Code Input and Output Files

Input File:

```

problem
  o/f=1.11
  rocket equilibrium
  ttest,k=3000
  p,psia=400
  sup,ae/at=20
react
  oxid=O2 wt=1 t,k=298
  fuel=HTPB wt=0.8200 t,k=298 h,kj/mol=-12.43 C 7.337 H 10.981 O 0.058
  fuel=AL(cr) wt=0.1764 t,k=298
  fuel=AL2O3(a) wt=0.0036 t,k=298
output
  siunits
  plot p t isp ivac m mw
end

```

Output File:

```

Pin = 400.0 PSIA
CASE =

```

	REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
OXIDANT	O2	1.0000000	-4.407	298.000
FUEL	HTPB	0.8200000	-12430.000	298.000
FUEL	AL(cr)	0.1764000	-3.630	298.000
FUEL	AL2O3(a)	0.0036000	-1675711.854	298.000

O/F= 1.11000 %FUEL= 47.393365 R,EQ.RATIO= 2.502418 PHI,EQ.RATIO= 2.514999

	CHAMBER	THROAT	EXIT
Pinf/P	1.0000	1.7671	229.82
P, BAR	27.579	15.607	0.12000
T, K	2977.80	2745.16	1090.71
RHO, KG/CU M	2.2046 0	1.3619 0	2.6794-2
H, KJ/KG	-76.373	-758.65	-4483.28
U, KJ/KG	-1327.35	-1904.57	-4931.15
G, KJ/KG	-35115.7	-33060.6	-17317.5
S, KJ/(KG) (K)	11.7669	11.7669	11.7669
M, (1/n)	19.792	19.918	20.249
MW, MOL WT	19.290	19.362	19.503
(dLV/dLP)t	-1.00642	-1.00373	-1.00757
(dLV/dLT)p	1.1426	1.0870	1.1235
Cp, KJ/(KG) (K)	3.5401	3.0086	2.6611
GAMMA _s	1.1744	1.1908	1.2303
SON VEL,M/SEC	1212.1	1168.1	742.3
MACH NUMBER	0.000	1.000	3.999

PERFORMANCE PARAMETERS

Ae/At	1.0000	20.000
CSTAR, M/SEC	1733.5	1733.5
CF	0.6739	1.7126
Ivac, M/SEC	2149.1	3119.7
Isp, M/SEC	1168.1	2968.8

MOLE FRACTIONS

*AL	0.00109	0.00058	0.00000
ALH	0.00037	0.00020	0.00000
*ALO	0.00006	0.00002	0.00000
ALOH	0.00513	0.00244	0.00000
AL(OH) 2	0.00001	0.00000	0.00000
AL2O	0.00152	0.00076	0.00000
AL2O2	0.00002	0.00000	0.00000
CH4	0.00000	0.00000	0.00083
*CO	0.54818	0.55081	0.54455
*CO2	0.00117	0.00058	0.00382
*H	0.01741	0.01067	0.00000
HCO	0.00002	0.00001	0.00000
*H2	0.39342	0.40303	0.41117
H2O	0.00616	0.00292	0.00284
*OH	0.00010	0.00002	0.00000
AL2O3 (a)	0.00000	0.00000	0.03054
AL2O3 (L)	0.02534	0.02793	0.00000
C (gr)	0.00000	0.00000	0.00626

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

ALC	ALC2	ALH2	ALH3	ALO2
AL(OH) 3	AL2	AL2C2	AL2O3	*C
*CH	CH2	CH3	CH2OH	CH3O
CH3OH	CH3OOH	COOH	*C2	C2H
C2H2,acetylene	C2H2,vinylidene	CH2CO,ketene	O(CH) 2O	HO(CO) 2OH
C2H3,vinyl	CH3CO,acetyl	C2H4	C2H4O,ethylen-o	CH3CHO,ethanal
CH3COOH	OHCH2COOH	C2H5	C2H6	C2H5OH
CH3OCH3	CH3O2CH3	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O,propylox	C3H6O,acetone	C3H6O,propanal
C3H7,n-propyl	C3H7,i-propyl	C3H8	C3H8O,1propanol	C3H8O,2propanol
C3O2	*C4	C4H2,butadiyne	C4H4,1,3-cyclo-	C4H6,butadiene
C4H6,1butyne	C4H6,2butyne	C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten
C4H8,tr2-butene	C4H8,isobutene	C4H8,cyclo-	(CH3COOH) 2	C4H9,n-butyl
C4H9,i-butyl	C4H9,s-butyl	C4H9,t-butyl	C4H10,n-butane	C4H10,isobutane
*C5	C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-
C5H11,pentyl	C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3) 2CH3
C6H2	C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol
C6H10,cyclo-	C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane
C7H7,benzyl	C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl
C7H16,n-heptane	C7H16,2-methylh	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene
C8H17,n-octyl	C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	HALO	HALO2
HCCO	HO2	HCHO,formaldehy	HCOOH	H2O2
(HCOOH) 2	*O	*O2	O3	AL (cr)
AL (L)	ALH3 (a)	AL (OH) 3 (a)	AL4C3 (cr)	H2O (cr)
H2O (L)				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

Appendix B: LGCP O₂ Test Data Sheet

LGCP O₂ TEST DATA SHEET

Test # _____		Date _____	
<u>Test Parameters</u>			
_____ %		Oxidizer flow est. _____ g/s	
_____ %		act. _____	
_____ %		O ₂ Reg. Press. _____ psi	
_____ %		O ₂ Pintle Pos. _____ in	
Fuel assembly mass _____		O ₂ Mass flow rate _____ g/s	
Preburn _____ g		Orifice size/CD _____ in	
Postburn _____ g		O ₂ Flux _____ kg/(m ² *s)	
		Test duration est. _____ s	
Fuel Length _____ in		act. _____	
Bore Preburn _____ in (dia)		Nozzle size _____ in (dia)	
Bore Postburn _____ in (dia)		N ₂ Purge Press. _____ psi	
		O ₂ Manifold _____ psi	
		N ₂ Purge Bottle _____ psi	
<u>Data Acquisition</u>			
Sampling rate _____ sec-1			
DAQ file name _____			
Pressure #1 _____	Channel _____	Pressure #3 _____	Channel _____
	Color Green		Color Blue
Pressure #2 _____	Channel _____	Pressure #4 _____	Channel _____
	Color Yellow		Color Red
<u>Comments</u>			
<u>Test Personnel</u>			

O2 Manifold Open	
O2 Manifold Shut	
O2 Run Open	
O2 Run Shut	
N2 Purge Open	
N2 Purge Shut	
Igniter Energize	
Igniter Deenergize	

Appendix C: LGCP Checklist for Motor Firing

CHECKLIST FOR O2 LGCP MOTOR FIRING

Oxygen LGCP Hybrid Rocket Motor Test Setup Procedure:

- ☐ Turn on the overhead fan and place a box fan near the run tank.
- ☐ Verify sufficient reserves of nitrogen and oxygen in bottles.
- ☐ Mount the outdoor test camera, install A/V lines.
- ☐ Setup a video camera and TV with a DVD recorder to record the motor firing.
- ☐ Title the DVD video display and set DVD to a new recording.
- ☐ Ensure proper size burst disk is installed.
- ☐ Verify the shop air is connected to all remotely operated valves and greater than 90 psig in room 127 (_____ psig).
- ☐ Plug in and turn on the power supply to patch panel. This is located beneath the mounting platform for the motor.
- ☐ Ensure all signal cables are connected and turn on the data acquisition system (Nicolet Vision).
- ☐ Verify sampling rate is 1 ks/s.
- ☐ Ensure all pressure transducers show appropriate baseline values on the data acquisition system (around 0psig +/-5).
- ☐ Ensure oxygen pintle on venturi is set to 2" (or full open).
- ☐ Ensure nitrogen purge line hand ball valve is aligned to LGCP.
- ☐ With the control board off, open the control program, "Hybrid Slab Motor Control V10.vi".
- ☐ Verify that program is in "Automatic" mode

- ☐ Start the program (upper left corner).
- ☐ Turn on the control board and ensure all valve indication and fuse lights are lit
- ☐ Ensure Oxygen run valve (light off) and nitrogen purge (light on) are shut.

Testing Procedure:

- ☐ Ensure all non-testing personnel are clear from the test cell and fenced-in area.
- ☐ Remove block from load cell.
- ☐ Open nitrogen purge bottle and set regulator to amount specified on test data sheet (~300psi greater than O2 regulator).
- ☐ Open reference pressure nitrogen bottle attached to oxygen regulator.
- ☐ Verify oxygen line hand valve and cluster hand valves with bottles are open (and hand valves leading to other systems are shut).
- ☐ Power on reference pressure digital readout.
- ☐ **Slowly** open oxygen bottle valves.
- ☐ Set oxygen regulator to value written on test data sheet (slightly lower)
- ☐ Insert the fuel grain, post-combustion chamber, and nozzle plug into the chamber.
- ☐ Insert the graphite filler pieces, electric match, and injector plug into the chamber.
- ☐ Make an announcement for starting the test firing: “We will be conducting a motor firing in room 127. Please stand clear of the test cell and the fenced-in area.”
- ☐ Connect igniter lines to electric match leads.
- ☐ Slid motor back so it is resting on load cell.
- ☐ Check ALL timing parameters.
- ☐ Re-check all regulators.
- ☐ Press “Record” on the DVD and start timer on title screen.

- ☐ Press “Record” on the data acquisition system.
- ☐ Press “Record” on Hybrid Slab Motor Control V.10.vi.
- ☐ Ensure all lights necessary for LGCP test are illuminated.
- ☐ Use the control program to initiate the test.

*****TEST INITIATED*****

- ☐ If misfire occurs, stop using this portion of checklist and move onto the Misfire Procedure section.

*****TEST CONCLUDED*****

- ☐ Press “Stop” on DVD recorder and data acquisition systems.
- ☐ Check that all valves have shut.
- ☐ Replace block for load cell.
- ☐ Disassemble motor, remove fuel grain, and secure injector plug to motor chamber.
- ☐ If additional tests are to be completed, move to the New Test section.
- ☐ Announce “We will now be venting gases in room 127, all personnel stay clear”.
- ☐ Secure the injector plug to the LGCP chamber.
- ☐ Close oxygen bottles at the cluster.
- ☐ With the igniter, fuel grain, and graphite pieces removed, using the manual mode of operation of the control program, open the oxygen run valve, wait a few seconds then allow manifold valve to vent.
- ☐ Close the oxygen run valve.
- ☐ Close nitrogen bottle purge bottle.
- ☐ Using the manual mode of operation of the control program, open the nitrogen purge valve to allow nitrogen lines to vent.

- ☐ Announce “Test completed in room 127”
- ☐ Close and vent the nitrogen regulator being used for O₂ pressure regulation.
- ☐ Check to ensure no back pressure in O₂ manifold.
- ☐ Turn off the patch panel power supply.
- ☐ Turn off O₂ reference pressure digital readout.
- ☐ Quit the Hybrid Slab Motor Control V10.vi control program.
- ☐ Turn off the control board.
- ☐ Close shop air ball valve in the machine shop.
- ☐ Replace block for load cell.

Misfire Procedure:

- ☐ Immediately turn off hybrid control board by turning key; this will start nitrogen flow and interrupt oxygen flow.
- ☐ Announce “Misfire has occurred in room 127, stay clear of the test cell and fenced in area until directed otherwise”.
- ☐ Continue nitrogen flow for at least 15 seconds.
- ☐ Continue recording event on outdoor camera.
- ☐ On the control program; restart and turn on manual mode and ensure all relays are in the shut position.
- ☐ Turn on control panel. Verify all flows have stopped and no smoldering is observed. If smoldering is observed, continue to purge the system using the manual control.
- ☐ Isolate oxygen by closing oxygen bottles at the cluster.
- ☐ Press “Stop” on the data acquisition system.

- ☐ Record time of misfire.
- ☐ Verify combustion has subsided via outdoor camera.
- ☐ After 10 minutes personnel may enter test chamber.
- ☐ Announce "Test completed in room 127".
- ☐ Gather evidence and determine cause of problem.

New Test:

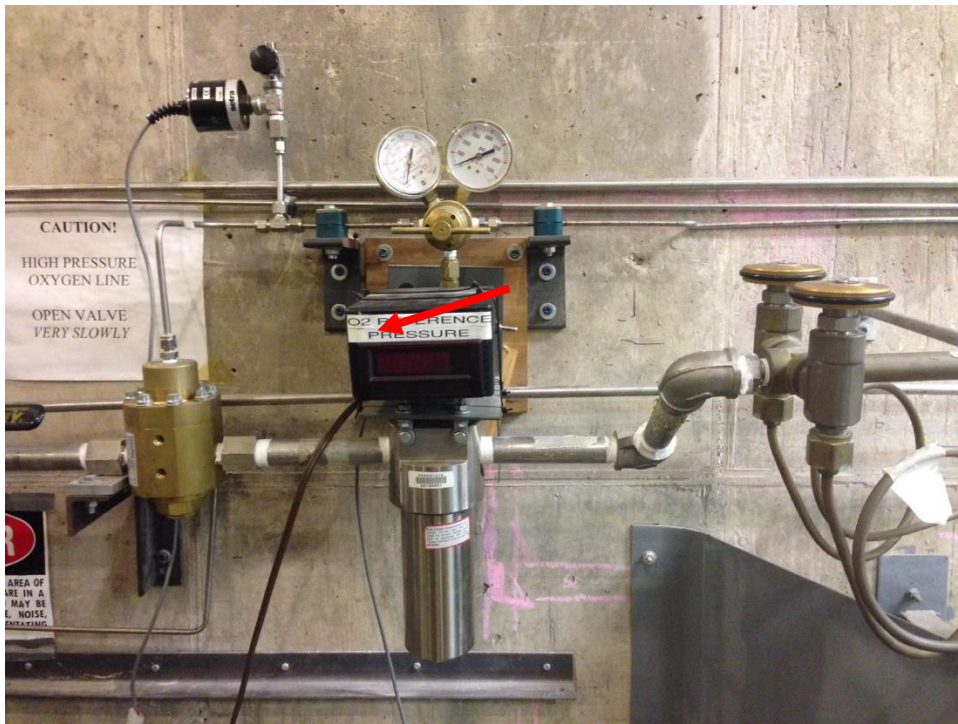
- ☐ Close oxygen hand valve.
- ☐ Close N2 Purge Bottle.
- ☐ Reload motor
- ☐ If next test is at a lower pressure vent O2 and N2 lines manually.
- ☐ Reopen O2 hand valve.
- ☐ Follow testing procedure for next test.

Appendix D: O₂ LGCP Motor Setup Walkthrough

Oxygen Tubing (in order):



Oxygen Manifold (RM 128)



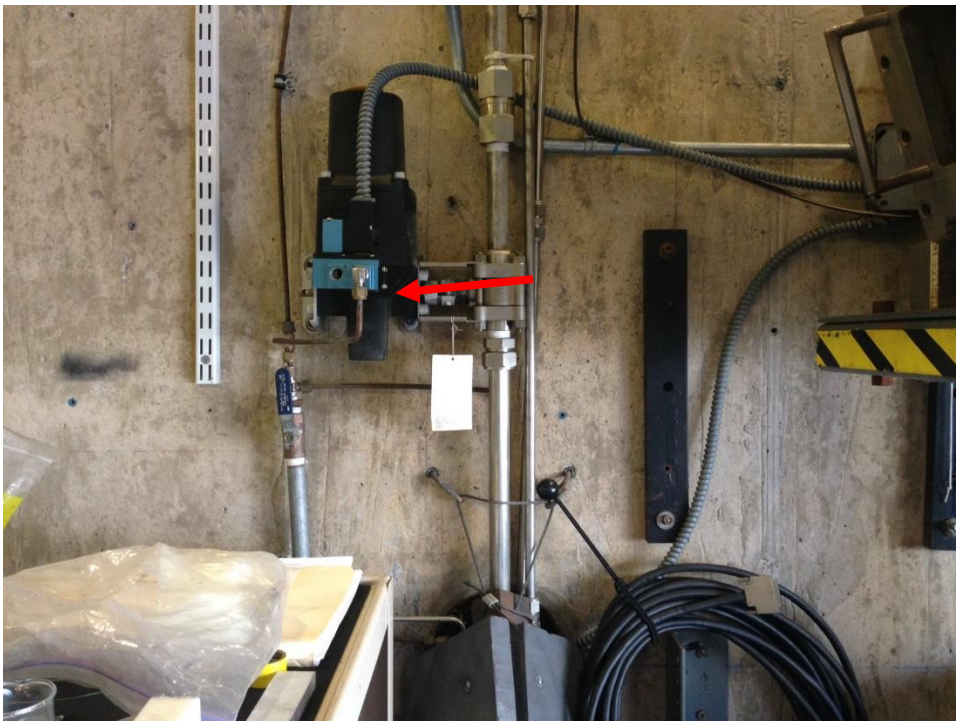
Oxygen Pressure Regulator (RM 128)



Oxygen Hand Valve (RM 128)



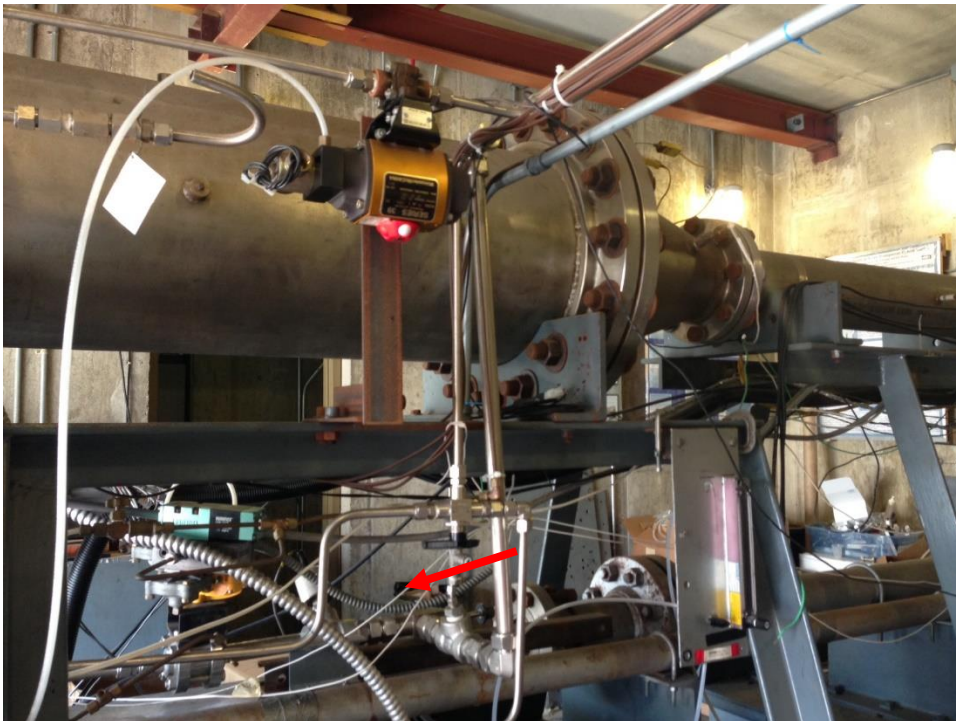
Nitrogen Reference for Oxygen Pressure Regulator (RM 128)



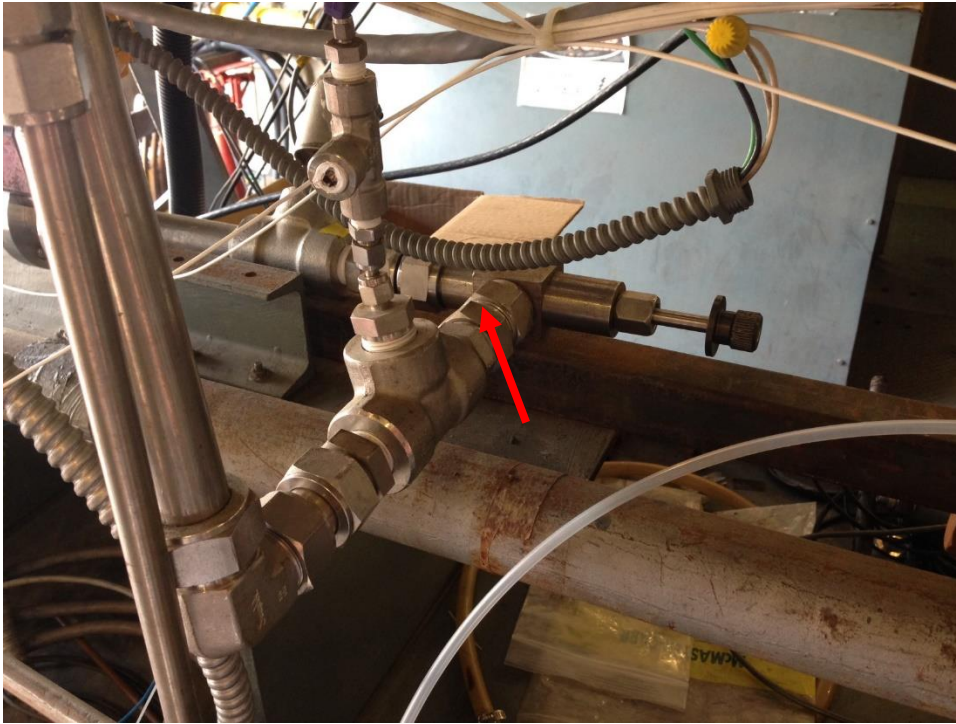
Oxygen Manifold Valve (RM 127)



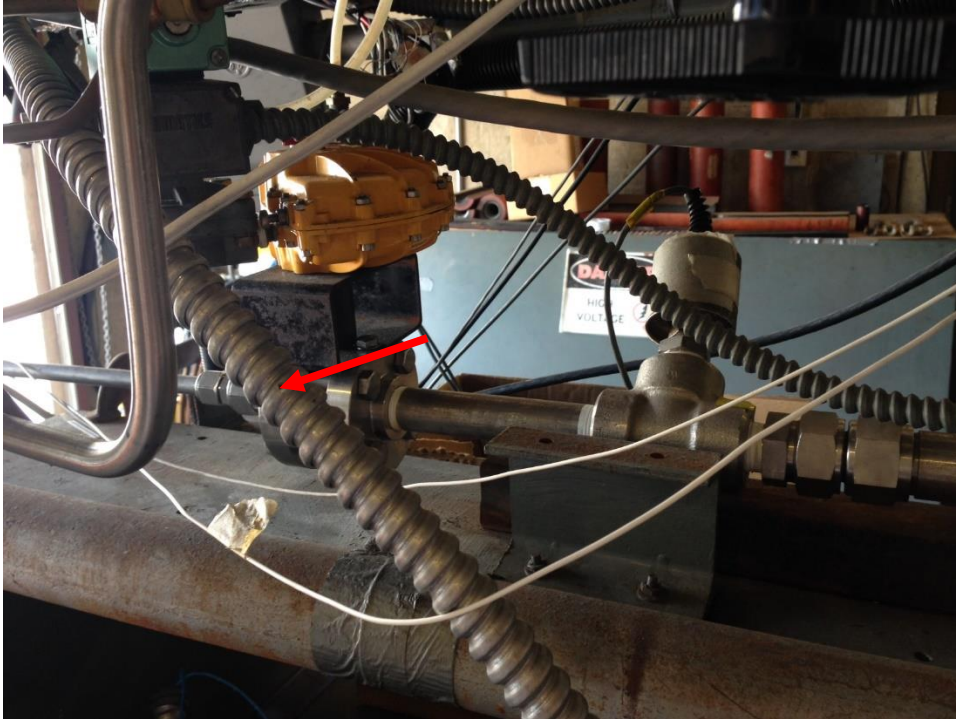
Oxygen Line (RM 127)



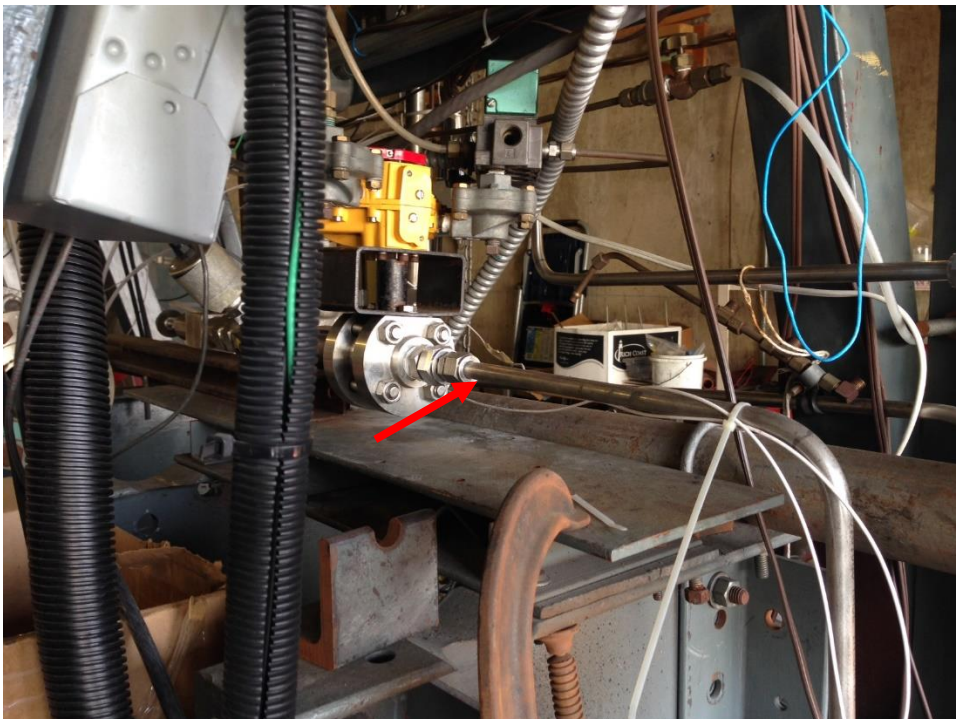
Oxygen Line (RM 127)



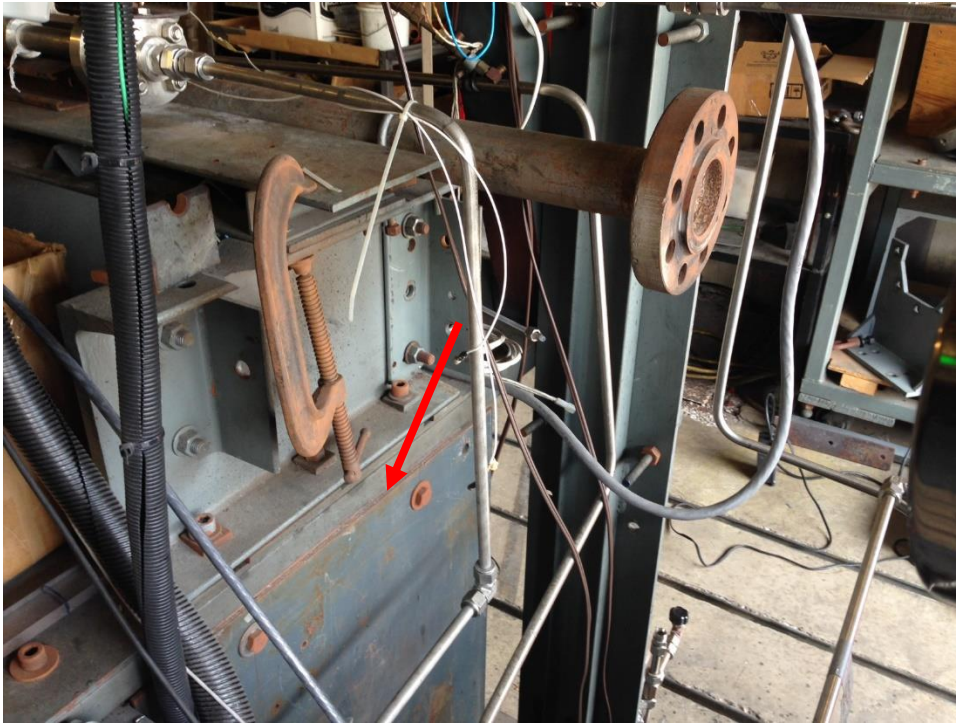
Oxygen Venturi Pintle (RM 127)



Oxygen Run Valve (RM 127)



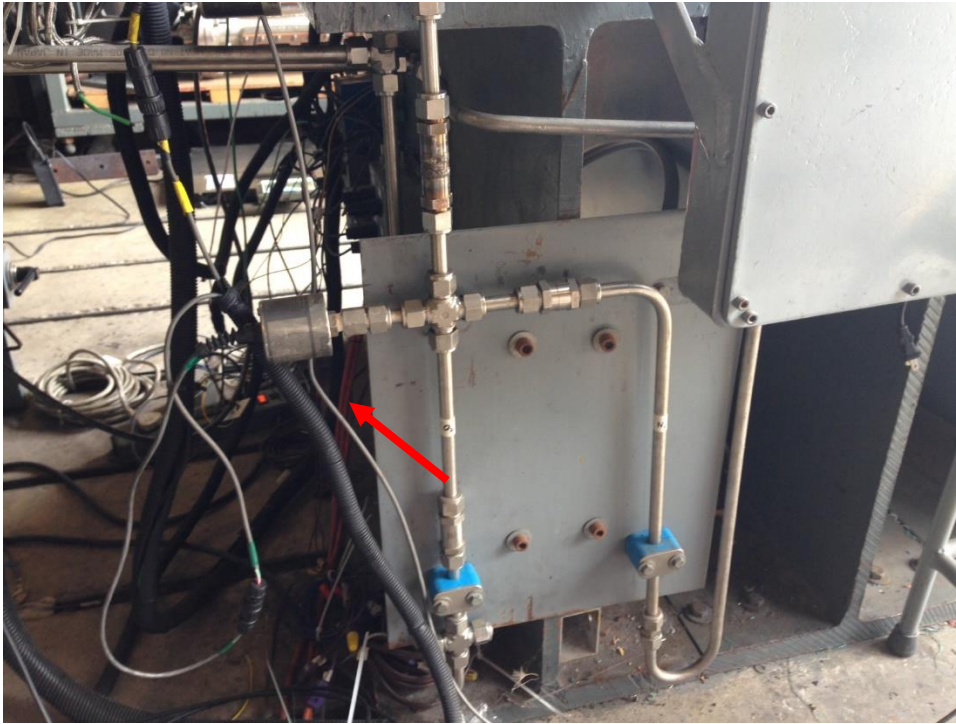
Oxygen Line (RM 127)



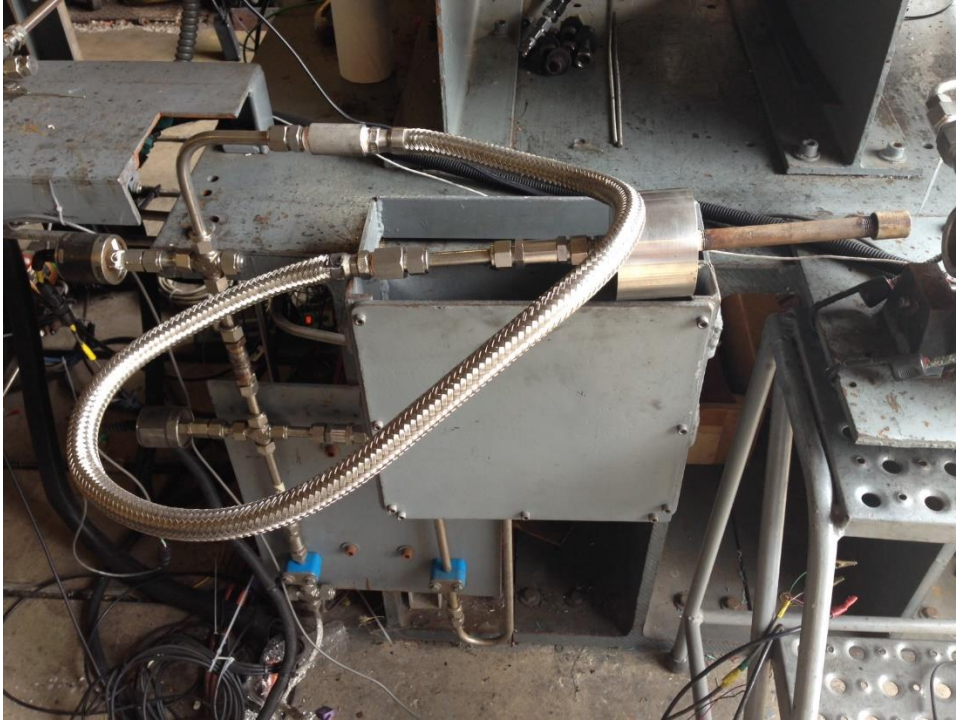
Oxygen Line (RM 127)



Oxygen Line (RM 127)



Oxygen into Orifice Setup (RM 127)

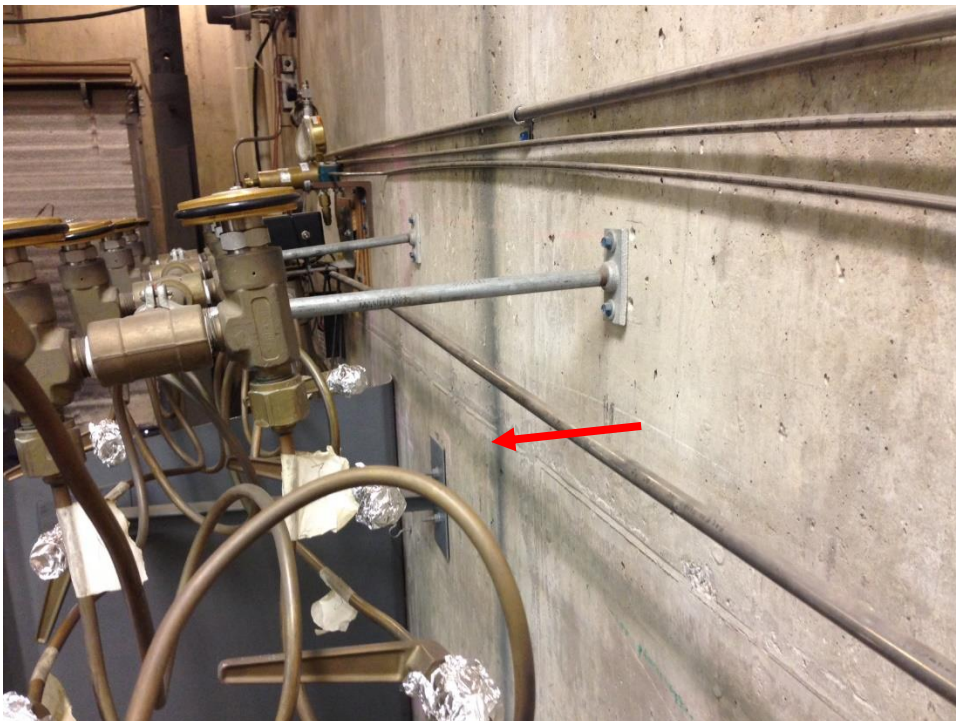


Oxygen into Motor (RM 127)

Nitrogen Tubing (in order):



Nitrogen Purge Bottle and Regulator (RM 128)



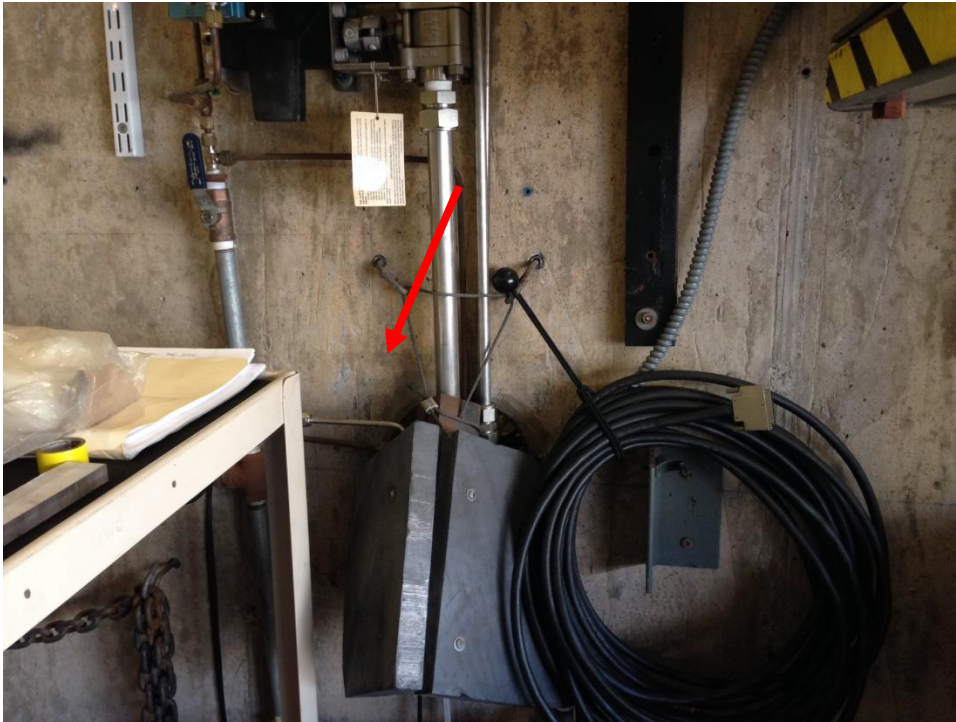
Nitrogen Line (RM 128)



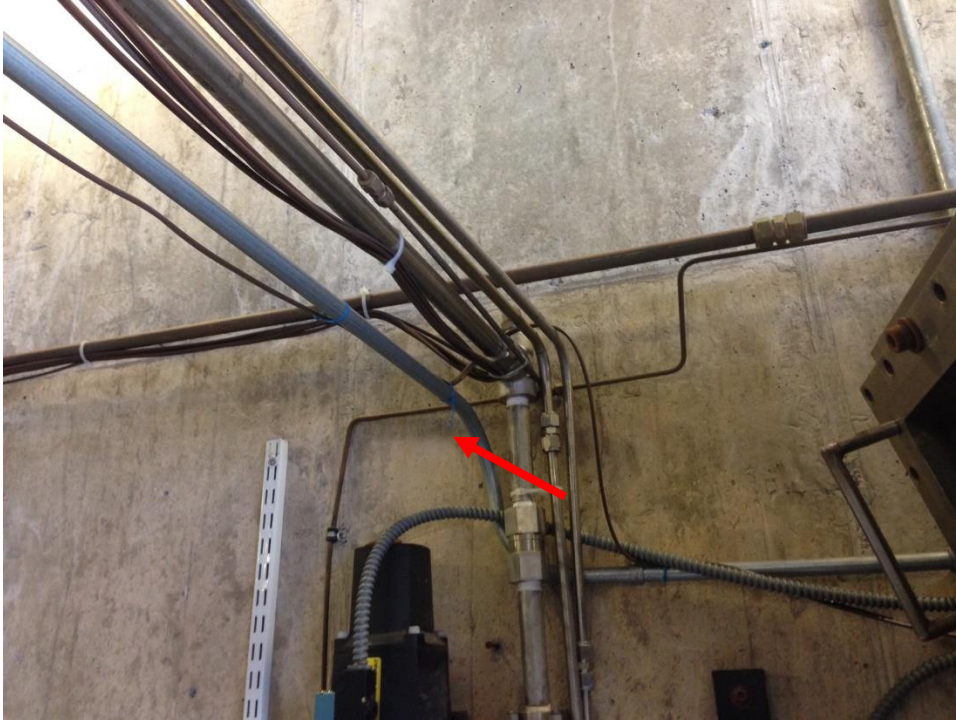
Nitrogen Purge Valve (RM 128)



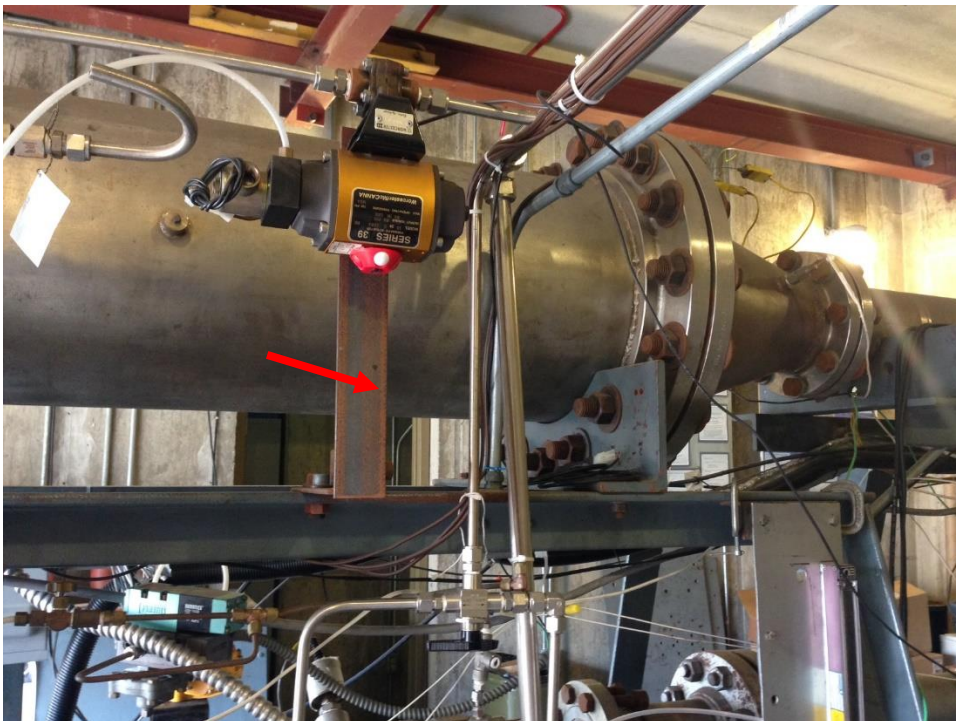
Nitrogen Line (RM 128)



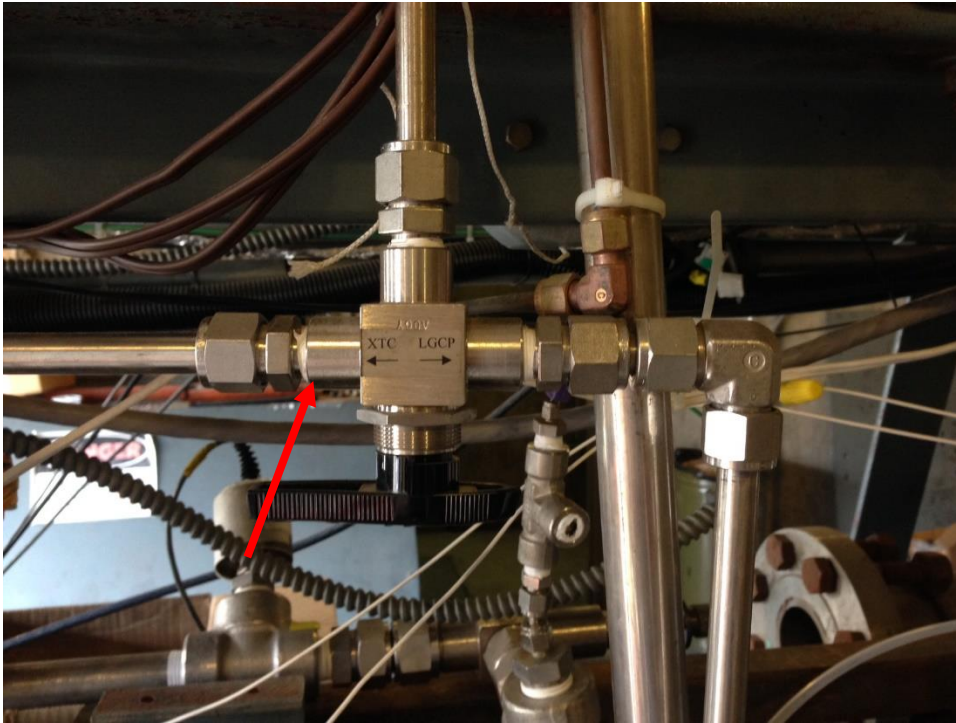
Nitrogen Line (RM 127)



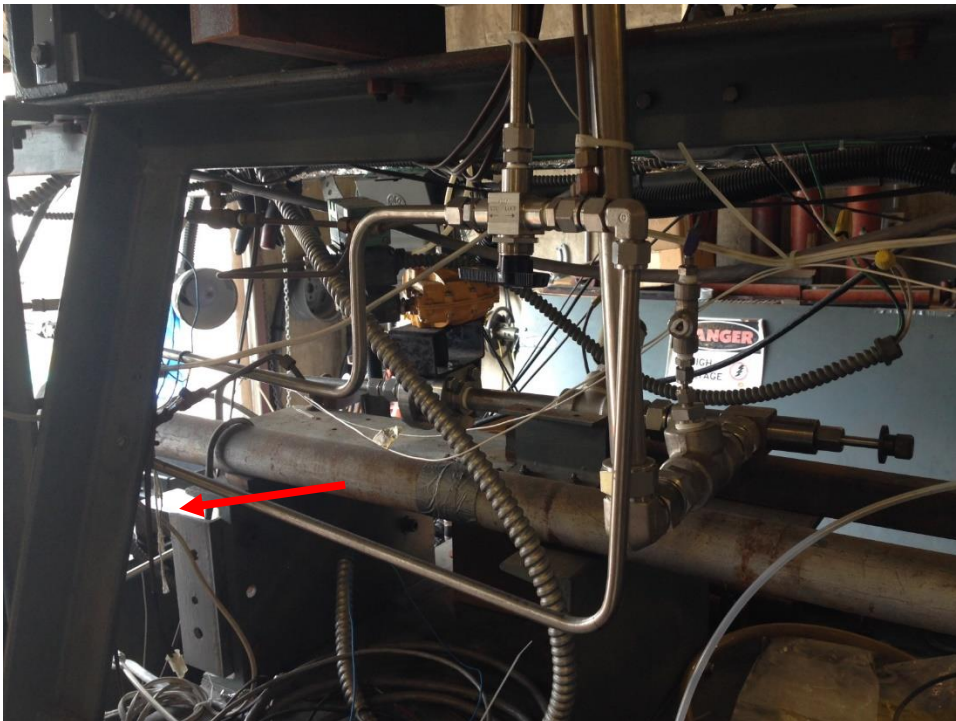
Nitrogen Line (RM 127)



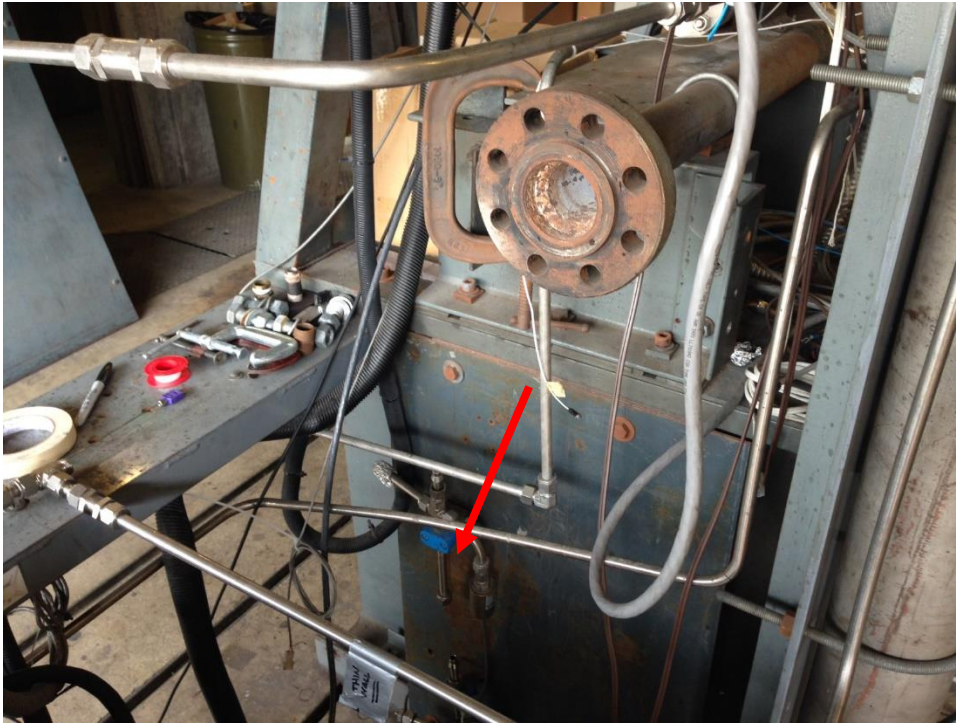
Nitrogen Line (RM 127)



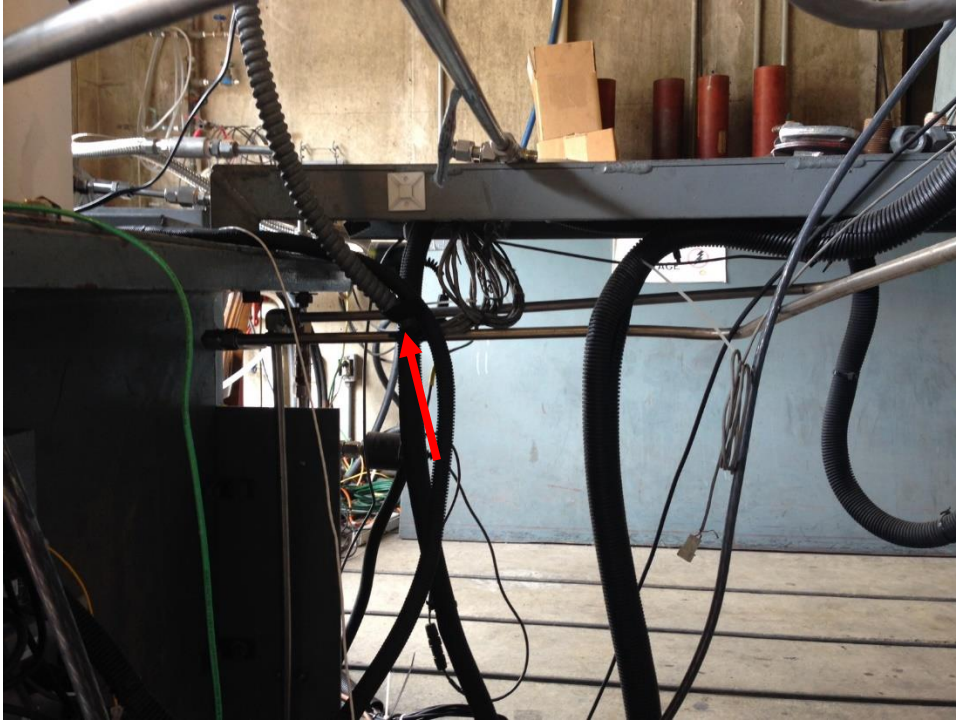
Nitrogen Ball Valve (RM 127)



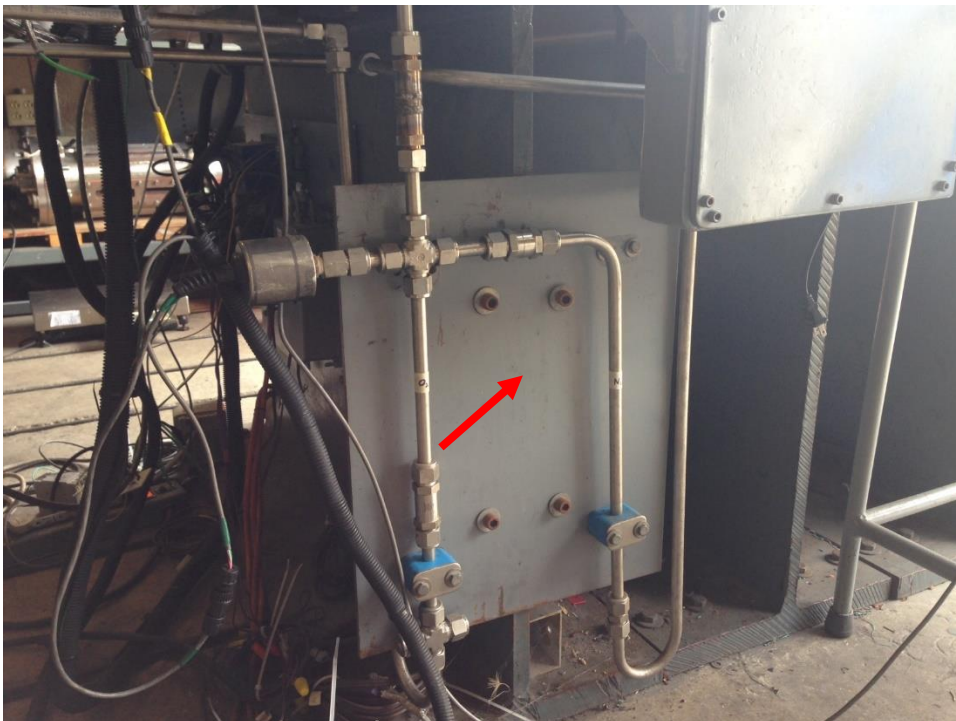
Nitrogen Line (RM 127)



Nitrogen Line (RM 127)



Nitrogen Line (RM 127)

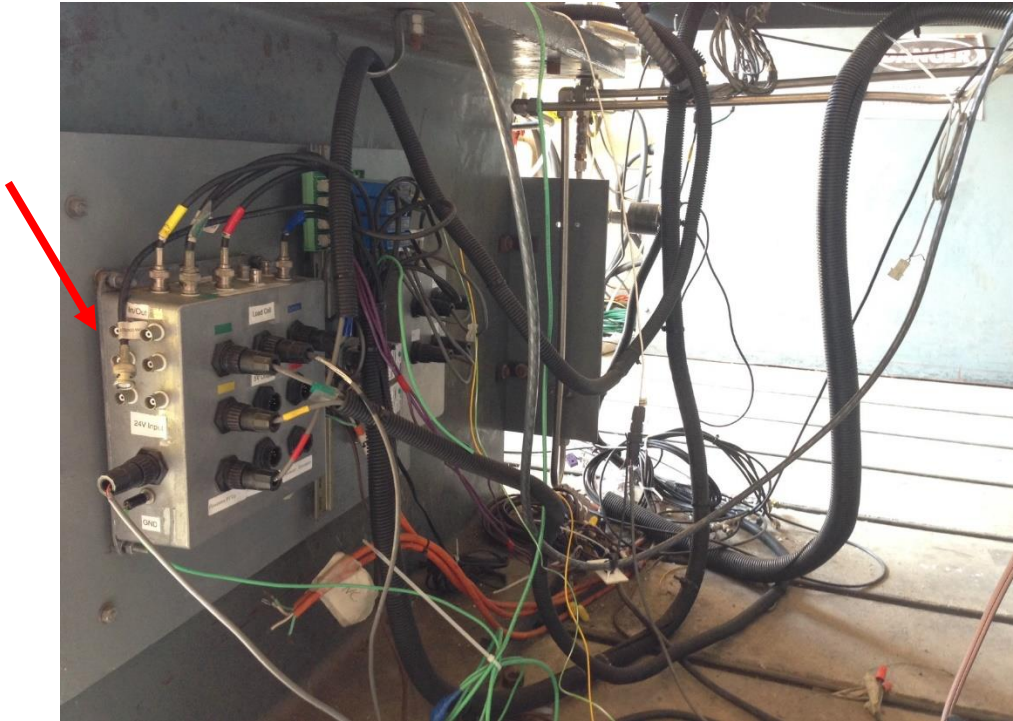


Nitrogen into Orifice Setup (RM 127)



Nitrogen into Motor (RM 127)

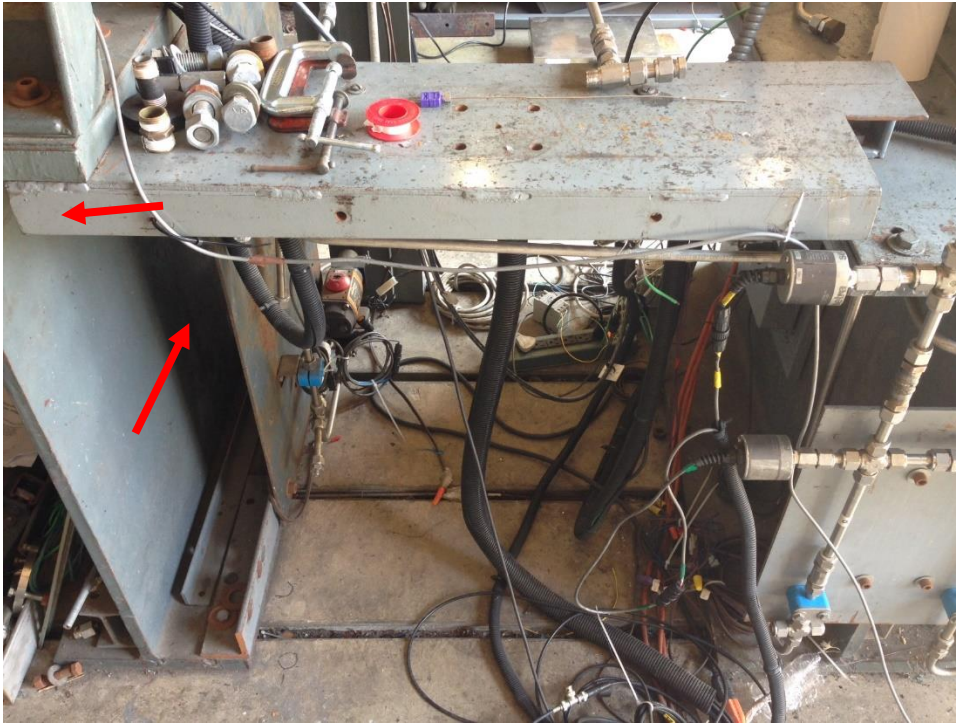
Electrical:



Panel for BNC Cables (RM 127)



BNC Wires (RM 127)



BNC and Igniter Wires (RM 127)



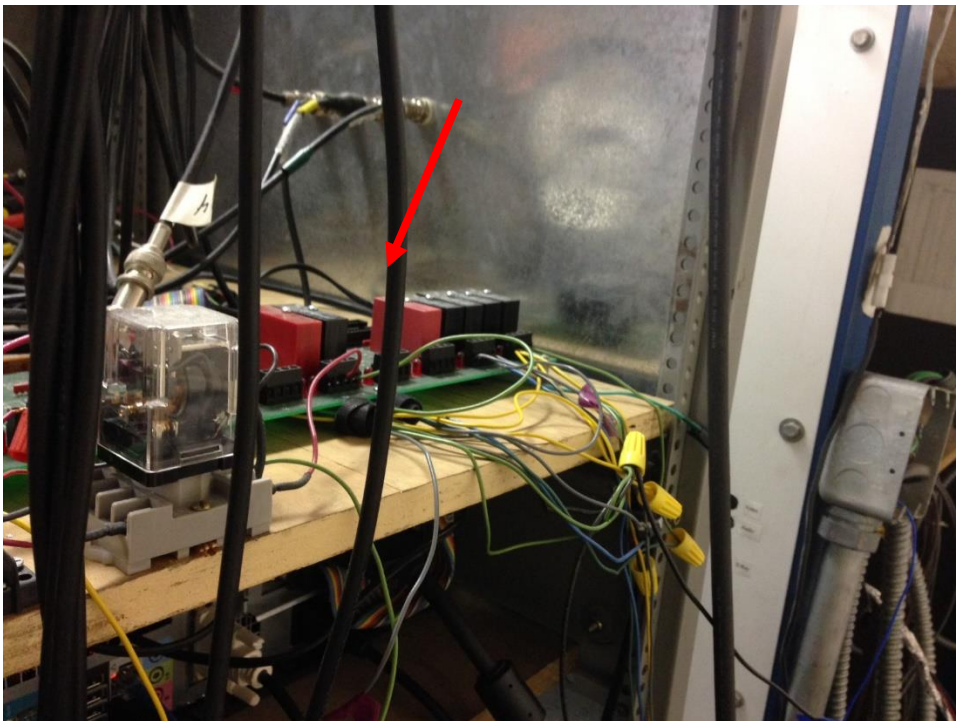
BNC and Igniter Wires (RM 127)



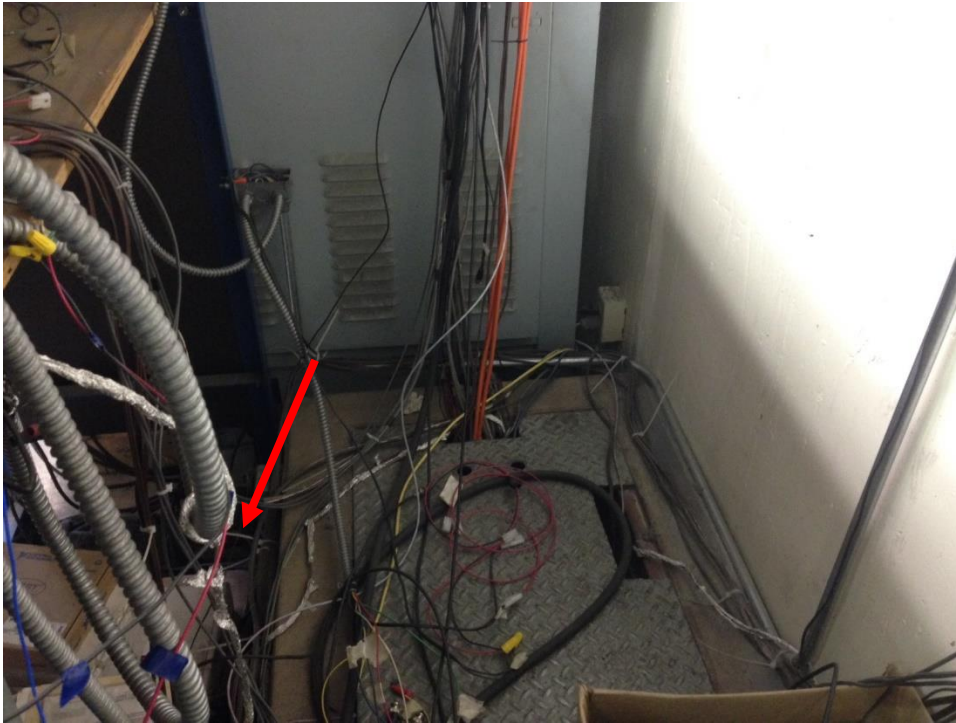
BNC and Igniter Wire Feedthrough to Control Room (RM 127)



BNC and Igniter Wire Feedthrough to Control Room (Control Room)



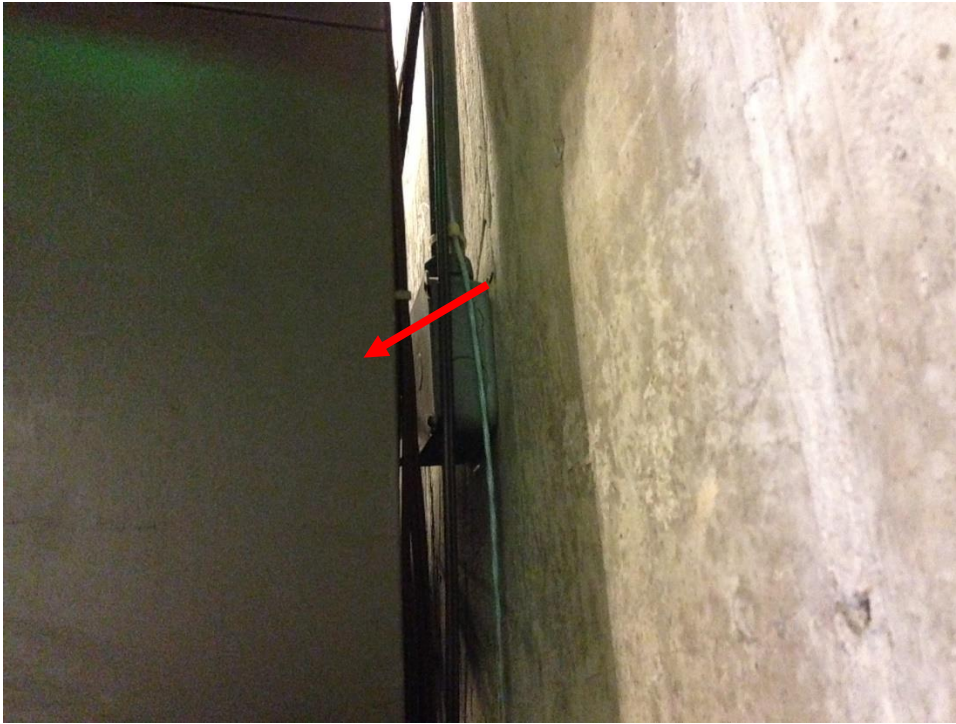
Relays (Control Room)



Relay Wires (Control Room)



Relay Wire Feedthrough Box (Control Room)



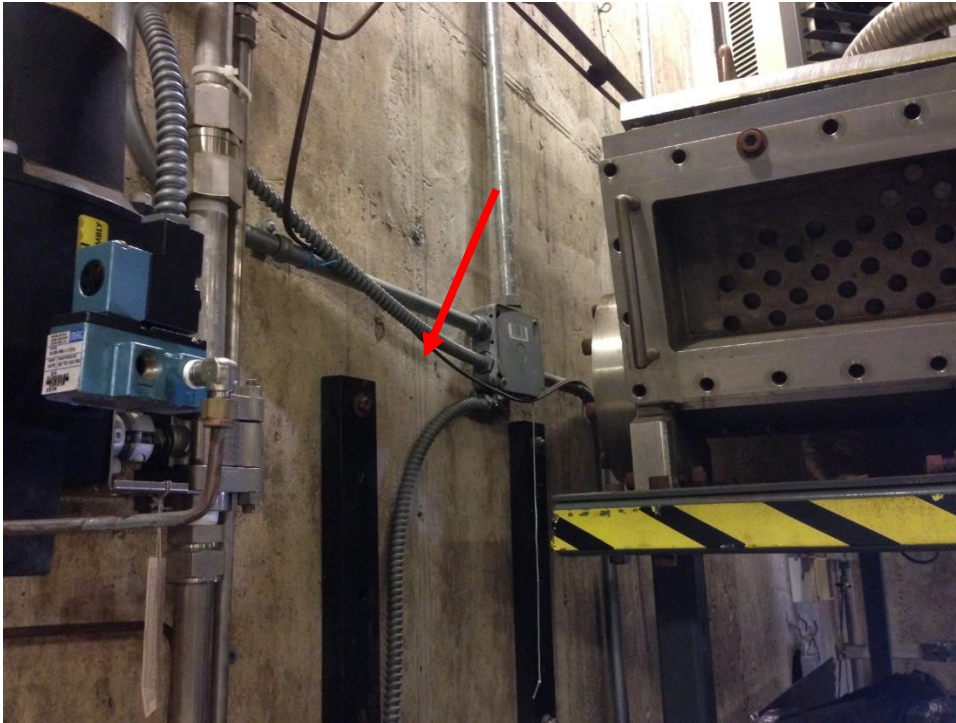
Relay Wire Feedthrough Box (RM 127)



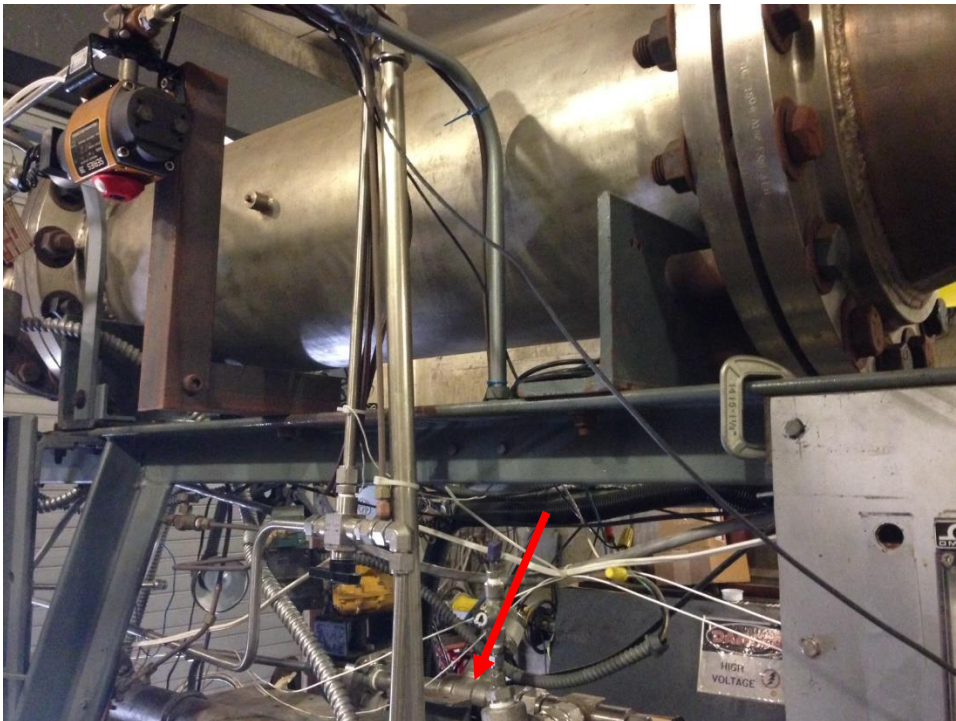
Relay Wires (RM 127)



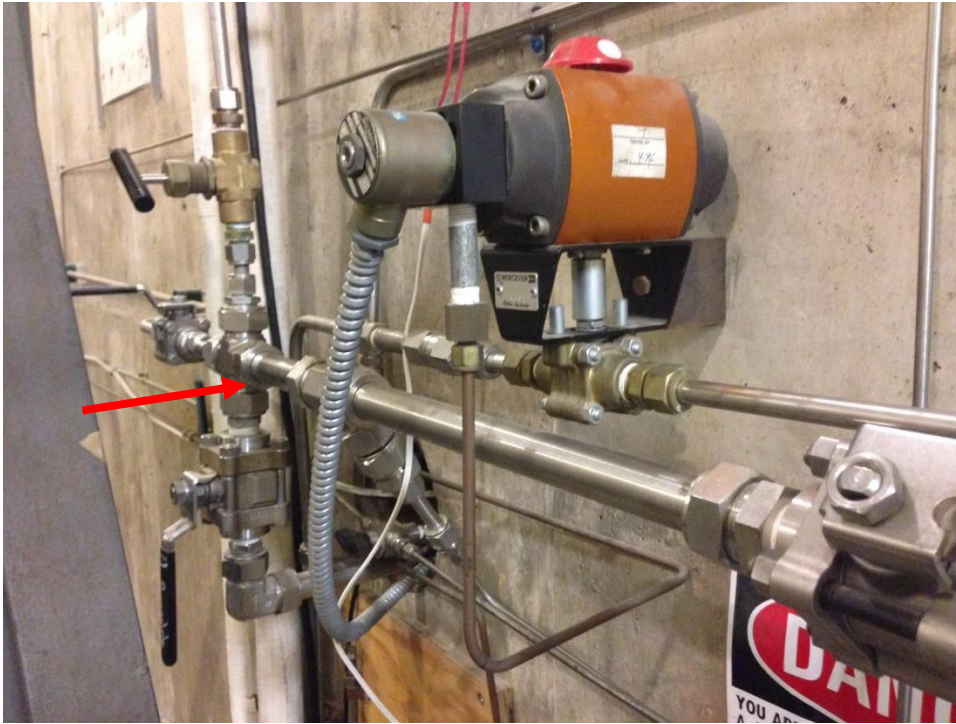
Relay Wires (RM 127)



Relay Wire Box to Valves (RM 127)



Relay Wires to Valve (RM 127)



Relay Wires to Valve (RM 128)

Appendix E: LGCP Firings of Aluminized Fuel Grains

The main focus of conducting experiments with the aluminized fuel grains with GOx was to obtain regression rates and combustion efficiencies for 18 and 40 wt% aluminum HTPB fuel grains. Two different aluminums were used for manufacturing the fuel grains: H30 from Valimet and X-85 from Toyal, both being 61.27 μ m in diameter. This gave the ability to see if there were any changes in regression rates and combustion efficiency between the two manufacturers. For the motor firings, an initial GOx value of 780 kg/m²s was required (one of the requirements for testing from NASA Jacobs) as well as a chamber pressure between 2.75-4.14 MPa (400-600 psia). The fuel length, oxidizer flow rate were all picked based upon the optimum O/F that corresponded to the highest I_{sp} . Figure E.1 below displays HTPB with aluminum loading up to 40% for a range of O/F values.

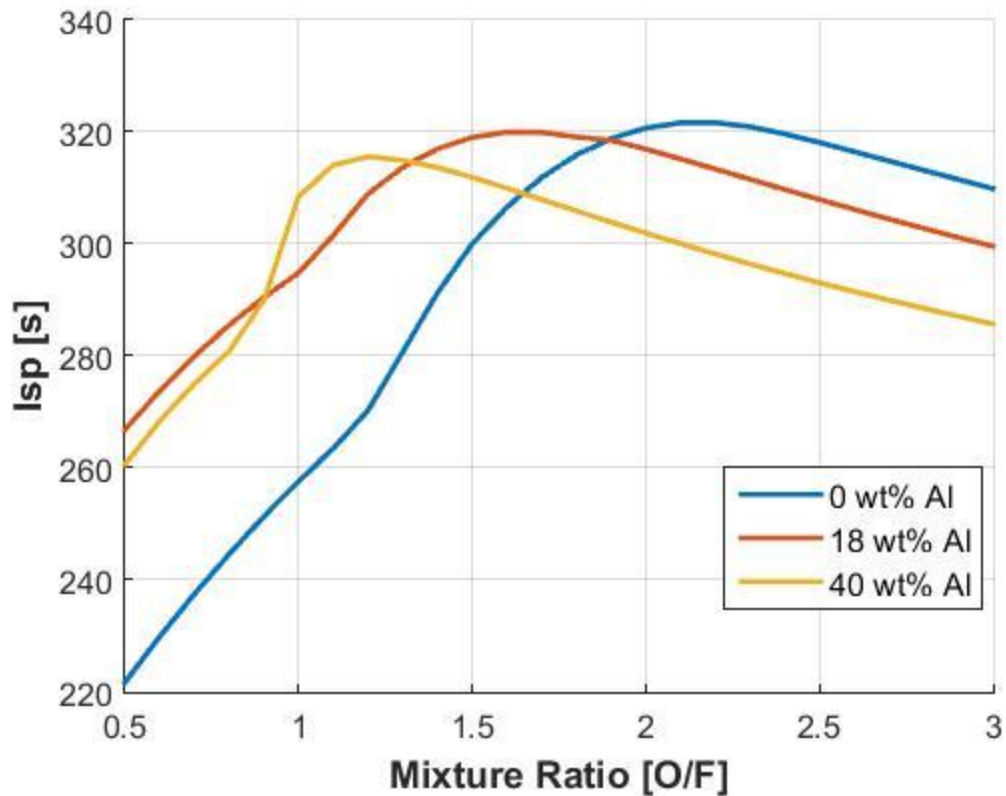


Figure E.1: HTPB aluminized fuel grains I_{sp} as a function of O/F.

Shown in Figure E.1 the optimum O/F for pure HTPB is 2, while it is 1.6 and 1.2 for 18 and 40 wt%, respectively. Given an initial GOx value and the optimum O/F, the fuel grain length can be calculated. The planning Excel sheet was used to calculate all the requirements for the rocket motor firings. After completion of each firing, the fuel grain was removed and inspected for even regression. After firing the first three fuel grains it was noticed that they were burning unevenly, with pockets of fuel gouging out of the center. This can be observed in Figure E.2 along with one actual rocket motor test that burned evenly.

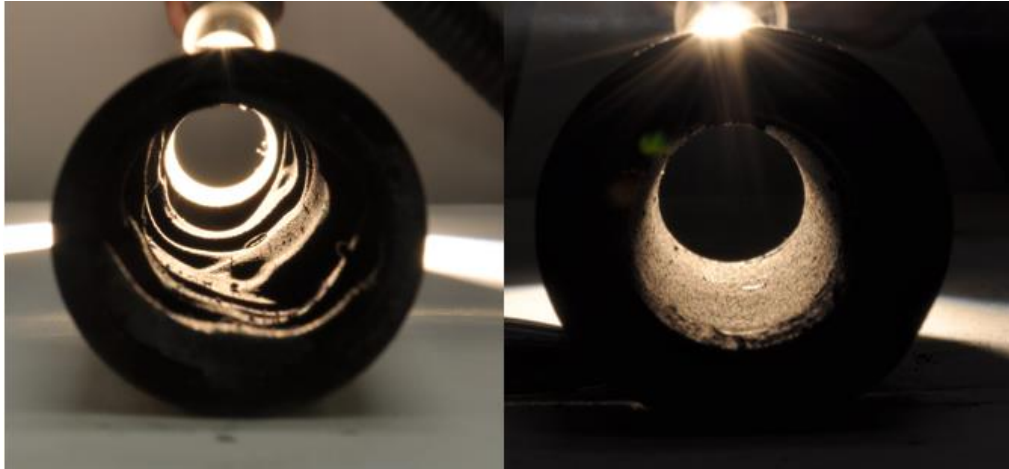


Figure E.2: Uneven and even post-burn of 18% aluminized fuel grains.

Due to this uneven regression, the fuel grains that were not tested were taken and X-rayed. Upon completion of X-raying the fuel grains it was found that the fuel grains had detachment issues as well as flaws. Below in Figure E.3 is an example of an X-ray image where the fuel grain appeared to be detached from the phenolic casing. To see if this was actually the case, that specific fuel grain was sectioned in half. Figure E.4 displays the sectioned fuel grain, where it is visible that the fuel grain was detaching away from the phenolic casing.

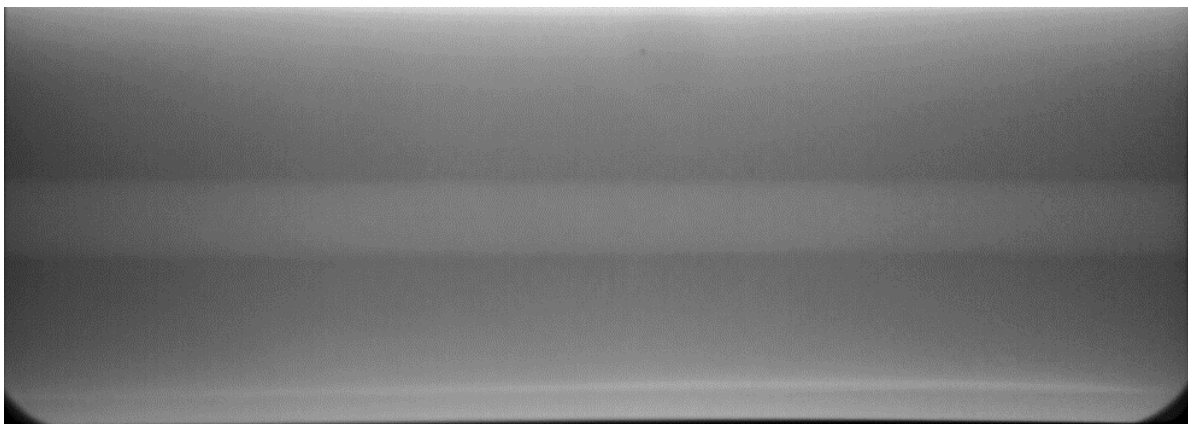


Figure E.3: X-ray image of detaching fuel grain away from phenolic tubing.



Figure E.4: Sectioned fuel grain that was X-rayed and found to be detaching away from the phenolic casing.

Not only were some of the fuel grains detaching, but there were radial flaws along the center port of the grain in Figure E.5. Again this fuel grain was sectioned, displaying the radial flaws that were discovered in the X-ray image in Figure E.6.

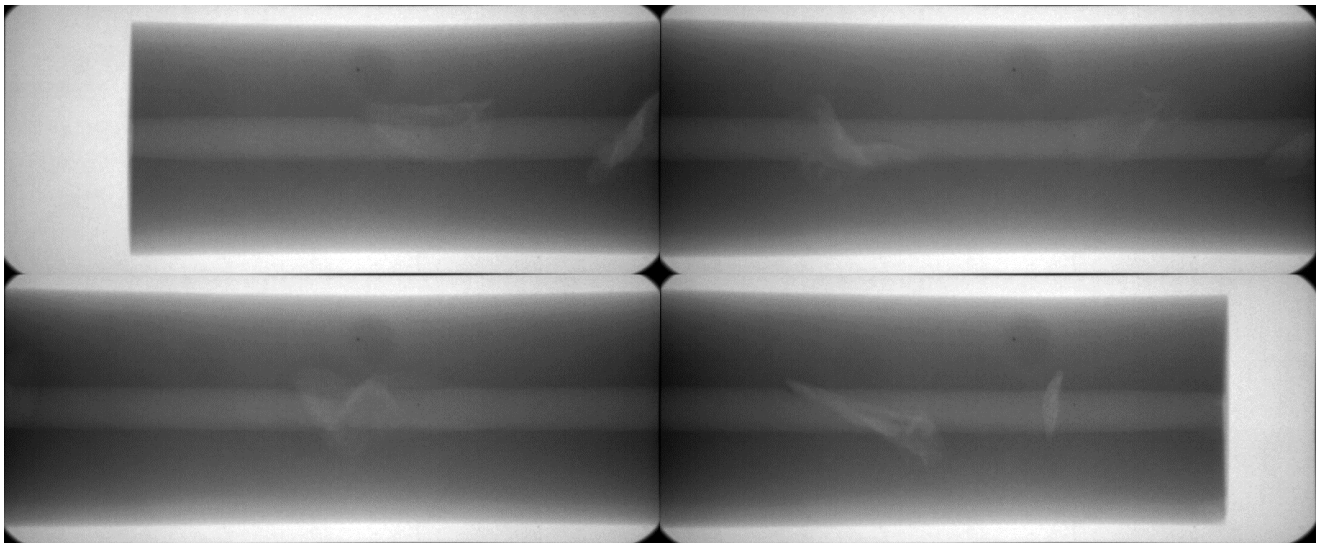


Figure E.5: X-ray image of fuel grain with radial flaws.

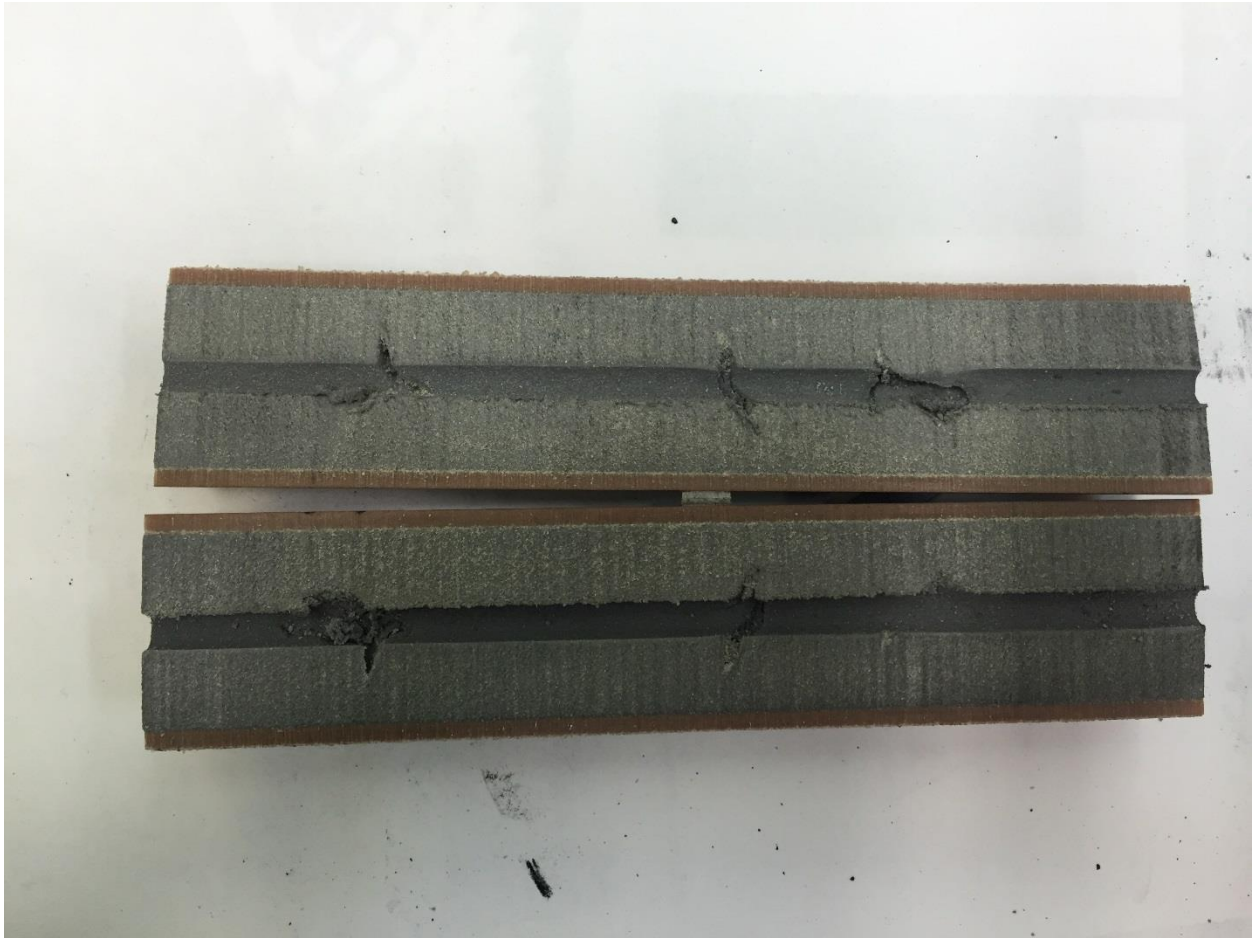


Figure E.6: X-rayed fuel grain in Figure E.5 taken and sectioned to display radial flaws.

To ascertain if the uneven burning rate was due to the flaws and detachment issues found from the X-ray imaging, two fuel grains were chosen to conduct a firing; one with no observed flaws in the X-ray images and one with flaws. It was hypothesized that the issues that were showing up with the uneven burning were due to the flaws from casting.

As hypothesized, the grain without any flaws seen in the X-ray images burned evenly while the one with flaws did not. Out of the eighteen grains sent to the HPCL, only seven were tested due to the issues found with the casting. The data were reduced and analyzed as described in section 4.2. With all of the uneven burning, however, it was hard to get accurate

measurements for the linear regression rate. This caused a significant amount of scatter in the data. A summary of the test results is provided in Table E.1. The resulting linear and mass regression rate data for the aluminized grains are plotted in Figure E.7 and Figure E.8.

Table E.1: Aluminized fuel grain test results.

NASA_SFT Test Results Summary								
Fuel	Length (in)	Avg. Chamber Pressure (psig)	Avg. O/F	Initial GOx (kg/m ² -s)	Avg. GOx (kg/m ² -s)	Avg. Regression Rate (mm/s)	Avg. Mass Regression (kg/s)	c* Combustion Efficiency
18% Al HTPB [627B-1]	5	340	2.745	744	68.2	1.43	0.008582	1.008
18% Al HTPB [627A-1]	5	289	2.42	737	96	1.36	0.009631	0.892
18% Al HTPB [627A-2]	6	265	2.54	743	121	1.195	0.009263	0.8334
18% AL HTPB [627B-2]	6	256	2.43	744	115	1.23	0.009683	0.7389
18% Al HTPB [627B-1]	12	584	1.11	745	123	1.119	0.02127	0.9578
18% Al HTPB [627A-1]	12	632	1.1	744.9	112	1.244	0.024122	0.9954
18% Al HTPB [627A-2]	12	539	1.17	739.01	112	1.14	0.0199	0.996
18% Al HTPB [627B-2]	12	514	1.52	750	110	1.08	0.02015	0.9617
18% Al HTPB [627B-3]	12	629	1.03	738	133	1.077	0.02263	1.01
40% AL HTPB [627C-2]	10.5	480	1.14	740	110	1.229	0.0205	0.88
40% Al HTPB [627D-1]	7	523	1.67	742	106	1.283	0.014	1.1

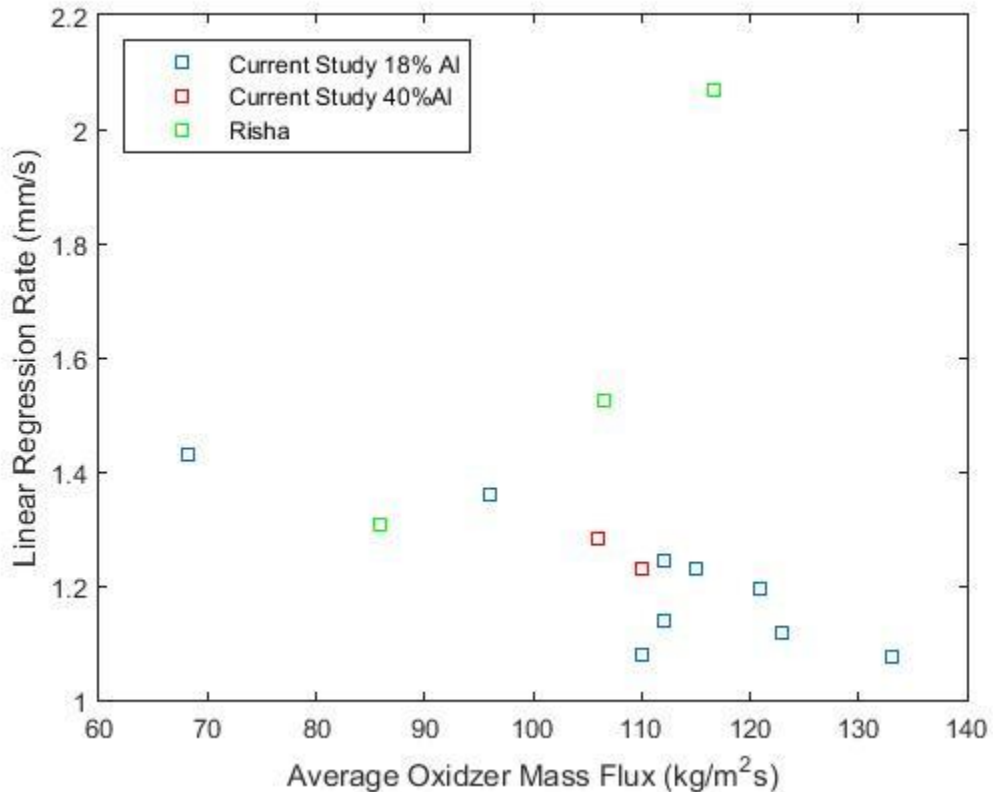


Figure E.7: Averaged linear regression rate for aluminized hybrid fuel grains with respect to the average oxidizer mass flux compared to Risha *et al.*

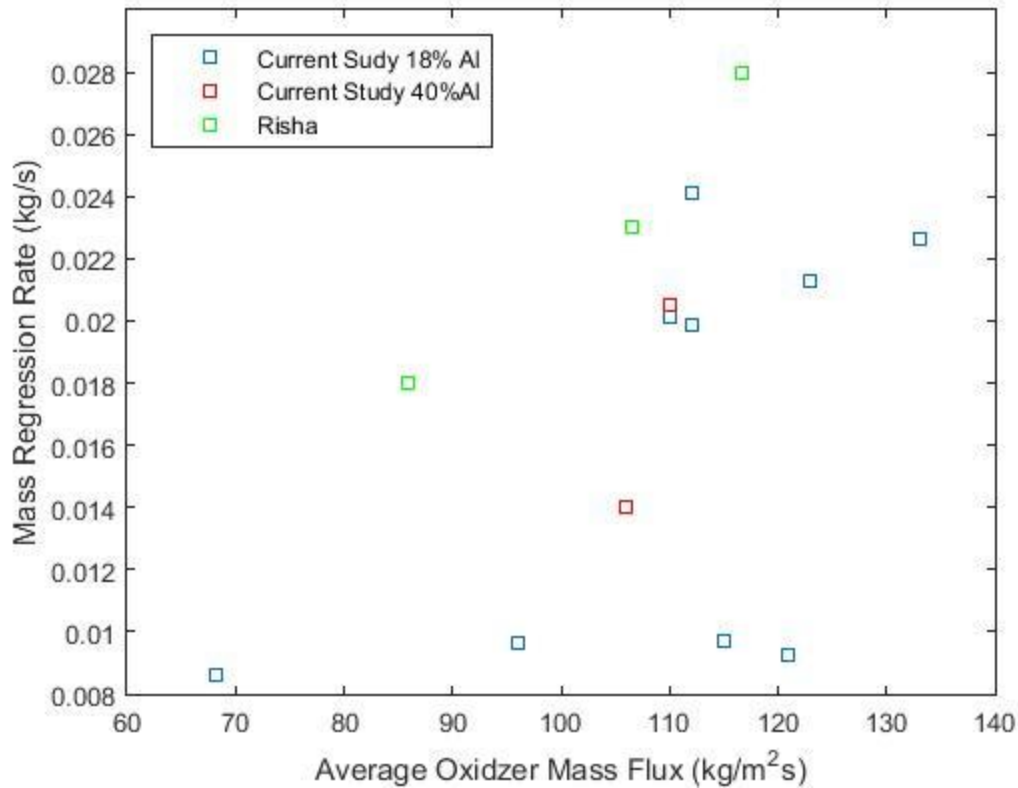


Figure E.8: Averaged mass regression rate for aluminized hybrid fuel grains with respect to the average oxidizer mass flux in comparison to Risha *et al.*

Although there was scatter in both the linear and mass regression rates, it comes close to the data collected from Dr. Risha who got the aluminum from a different manufacturer in a slightly smaller size, NTECH-50 nm at 20 wt% [4]. However, the data are inconclusive. The linear regression rate decreases as the oxidizer mass flux is increased. The linear regression rate should be increasing with increasing oxidizer flux, as seen with Risha. The mass regression rate seems to be a more viable option given the fact that the mass was measured for pre and post-test, however, there is too much scatter in the data to make any conclusions and comparisons.

Therefore, since the fuel grains mass was measured pre- and post-testing the mass average burning rate was converted to a linear burn rate. This still proved to be unreliable due to

the scatter and again, yielded a decrease in linear regression rate with increase in GOx, seen in Figure E.9.

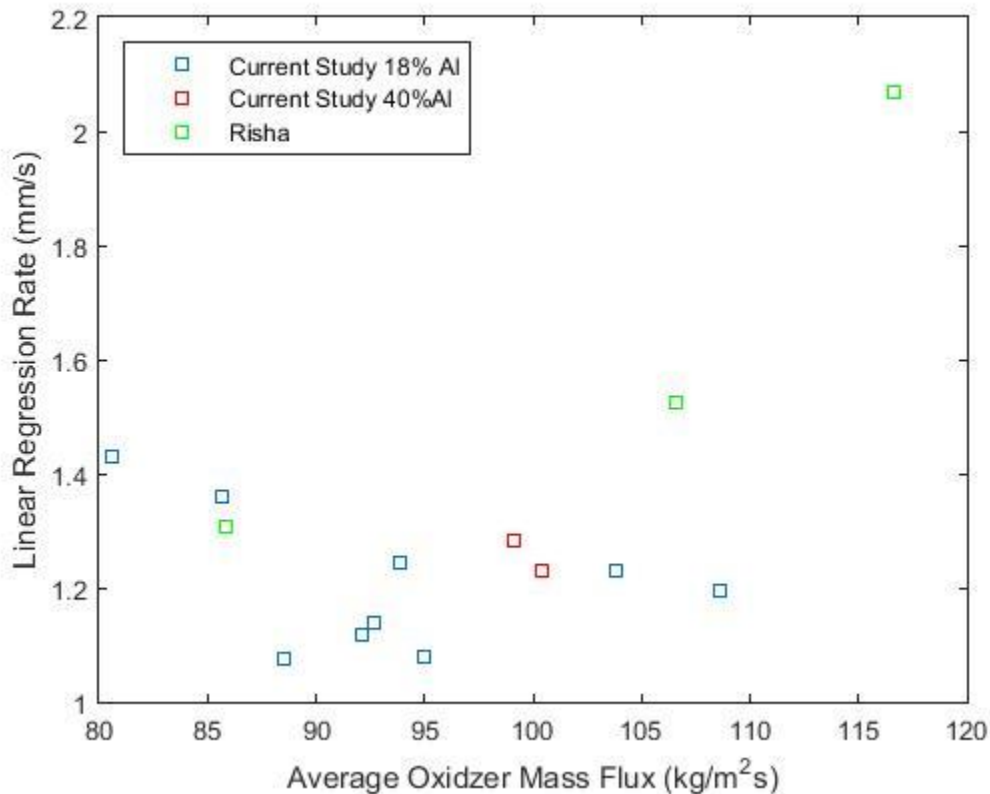


Figure E.9: Averaged linear regression rate determined from the mass regression rate for aluminized hybrid fuel grains with respect to the average oxidizer mass flux.

Although the data were unreliable and did not come to any significant conclusions, it was found that the fuel grains exhibiting flaws in the X-ray images were the ones with uneven burning. This shows the overall major benefit of a hybrid rocket motor, safety. Even though no data was determined from the testing, the actual rocket motor itself did not malfunction due to the flaws in the fuel grain; similar flaws in a solid propellant grain would have resulted in a potentially damaging overpressure or explosion.

Appendix F: Octave Wrapper Code

```
%Paige Nardozzo
%Start Date: 11/30/2105
%End Date: 2/28/2016
%PROGRAM: CHEMKIN_opposed_flow
%PURPOSE: Entry point for the console application

clear
clc
more off %since Octave doesn't display stuff within the while loop until it is finished
        %use more off to make sure it goes straight to the screen and displays everything
        %while it is running.

%Execution parameters and other user settings
maxloops = 5;
%Ti = 298 ;%initial temperature (k)

%Set filenames to use
%therm_data_file = 'therm.dat' ;%Therm file name
%therm_output_file = 'therm_output_file' ;%Therm output filename
%trans_data_file = 'trans.dat' ;%Trans data file
%trans_input_file = 'trans_input_file' ;% transport data file
%trans_output_file = 'trans_output_file' ;%trans output file
%chem_input_file = 'chem_input_file' ;%chem input file
%chem_output_file = 'chem_output_file' ;%Chem output file
%oppdiff_input_file = 'OppDiff-HTPB_N2O.inp' ;%premix input file

%***Start body of program***
%*Initialize shell environment

[N, R, Q, F] = Set_CHEMKIN_env () % Function for setting up the environment variables for CHEMKIN

%*Initialize variables
delta_rb = 1e0; %Initialize to some huge value so convergence loop runs...
rb_tol = 1e-6;

loopcount = 0 ;

error_message = ""

%* Preprocess chemistry meachansim, therm, and transport data files
% Preprocess chem.inp mechanism file and therm.dat data file (this is explained
% in "Getting Started 4.3")
% status = system('%REACTION_DIR%\chemkin15141_win64\bin\chem -i chem.inp -o chem.out
% & -d %REACTION_DIR%\chemkin15141_win64\data\therm.dat')

% [status,cmdout] = system('%REACTION_DIR%\chemkin15141_win64\bin\chem -i Glarborg_hc_no_reburn.inp
-o Glarborg_hc_no_reburn.out -d %REACTION_DIR%\chemkin15141_win64\data\therm.dat')
[status,cmdout] = system('%REACTION_DIR%\chemkin15151_win64\bin\chem -i Glarborg_hc_no_reburn.inp -o
Glarborg_hc_no_reburn.out -d %REACTION_DIR%\chemkin15151_win64\data\therm.dat')
disp('Preprocessed chemistry and therm data files....')
```

```

%Preprocess tran.dat file

%[status,cmdout] = system('%REACTION_DIR%\chemkin15141_win64\bin\tran -o tran.out -d tran2.dat')
[status,cmdout] = system('%REACTION_DIR%\chemkin15151_win64\bin\tran -o tran.out -d tran2.dat')
disp('Preprocessed transport data file')

%***Main loop - checks rb match for convergence between assumed value and calculated
%value from gas phase heat transfer
%Put in a do loop/while loop to make sure that it keeps on iterating if delta_rb>rb_tol
while abs(delta_rb>rb_tol)

%Check to see if maximum number of loops reached loopcount is acting
%strange and i set it to start at 0 but autamtically jumps to 1 but it used
%the case to run the opposed flow burner of loopcount=0 is this a problem?

if (loopcount==maxloops)
    X = ['Loopcount=', num2str(loopcount)];
    disp(X) %other parameters of interest for problem-solving
    error_message='Maximum loopcount reached with no convergence.'
    break
endif

% ** Run opposed flow burner diffusion CHEMKIN program
if (loopcount==0)
    %run PREMIX to find new solution
    [status,cmdout2] = system('%CHEMKIN_BIN%\CKReactorOpposedFlow -i OppDiff_HTPB_N2O22.inp -o
OppDiff_HTPB_N2O22.out')
    disp('CKReactorOpposedFlow executed')
    elseif %if loopcount>0 run PREMIX with restart file and new input file
    [status,cmdout3] = system('%CHEMKIN_BIN%\CKReactorOpposedFlow -i OppDiff_HTPB_N2O22.inp -o
OppDiff_HTPB_N2O22.out')
    disp('CKReactorOpposedFlow with restart executed')
endif

%Check for succesful execution

%Check for existence of XMLDate.zip file
C = exist('XMLData.zip', 'file')
if (C == 0)
    disp('No XMLData.zip file exists...please check input files and output')
    disp('logs for possible errors, then restart')
    error_message = 'Missing XMLData.zip'
    break
endif

%Check for existence of executuable output logfile and look for signs of success
D = exist('OppDiff_HTPB_N2O22.out','file')
if (D == 0)
    disp('No oppdiff.out file exists please check input files and output')
    disp('logs for possible errors, then restart')
    error_message = 'Missing output logfile'
    break
endif
%Check for indication of successful convergence in CHEMKIn app output file:

```

```

%'TWOPT: SUCCESS. PROBLEM SOLVED.' seen at end of output for good run,
%so search for substring with this line.
%*be careful with this--look at some output files to make sure it doesn't
%converge, refine the grid, then *not* converge for final case. May need to
%go to end of output file, rewind a few lines, and scan them to make sure
%only final status of TWOPT is captured

%Pattern = 'TWOPT: SUCCESS'
%A = fileread('OppDiff_HTPB_N2O.out')
%B = strfind(A,Pattern)
%empty = [] %what B will spit out an empty matrix if the pattern is not
           %found in the file

%if isequal(size(empty), size(B))
%disp('No TWOPT success found...may be a convergence problem')
%error_message = 'No TWOPT: SUCCESS found'
%break
%else %if the B matrix is not empty
%disp('TWOPT appears to have been successful! Continuing...')
%endif

%*Extract solution data from XMLData.zip output file
%By default, GetSolution writes to comma-delimited row based file
%CKSoln.csv (see "Getting Started" 4.4) also run CKSolnTranspose
%to create columnar data to simplify reading. Unless full paths supplied,
%XMLData.zip and CKSolnList.txt preferences must be in working directory
%Hand modify CKSolnList.txt to produce only data needed for coupling the
%the interface

disp('Checking Solution...')

%Check for CKSolnList.txt prefs file--if doesn't exist, generate a "new"
%one based on solution and stop for modification
%% Check to see if it works without rerunning entire license and everything
%FIX THIS SO IT WORKS!!!
%Added 12/3/15
E = exist('CKSolnList.txt','file')

if (E == 0)
    disp('Cannot find CKSolnList.txt file')
    disp('Please edit a txt file to include relevant parameters and species')
    disp('to match those read in the OppDiff code')
    %shell_cmd = 'GetSolution -listonly XMLData.zip' %Generate generic prefs file
    %[cmdout4] = Run_shell(shell_cmd)
    disp('Please modify file and re-run program')
    disp('Hit <Enter> to exit')
    error_message='Generic CkSolnList.txt created'
    break
endif

%Process output data in XML_zipfile using prefs file
%[status,cmdout] = system('%REACTION_DIR%\chemkin15141_win64\bin\tran -o tran.out -d tran2.dat')
[shell_cmd, cmdout5] = system('%REACTION_DIR%\chemkin15151_win64\bin\GetSolution
Z:\users\Paige\CHEMKIN_Burn_Rate\XMLData.zip') %-listonly messed up and only produces the CKSolnList File

```

```

    %[shell_cmd, cmdout5] = system('%REACTION_DIR%\chemkin15141_win64\bin\GetSolution -p
CKSolnList_Thermal_Conductivity.txt Z:\users\Paige\CHEMKIN_Burn_Rate\XMLData.zip') %-listonly messed
up and only produces the CKSolnList File
    %[cmdout4] = Run_shell(shell_cmd)

%Transpose row lists in CKsoln.csv into columns
%By default, creates a set of column-based *.csv files
%(see "Getting Started" 4.4). Unless full paths supplied, CKSoln.csv
%must be in working directory
[shell_cmd, cmdout6] = system('%REACTION_DIR%\chemkin15151_win64\bin\CKSolnTranspose')
%[cmdout4] = Run_shell(shell_cmd)

%Get data out of excel spreadsheet
%Added 12/4/15
%Make sure these variables and order match those in CKSolnList.txt
%Use csvread to obtain the values in CKSoln_solution_no_1_1

Temp_1 = csvread('CKSoln_solution_no_1.csv', 'C2..C2') %K
Temp_2 = csvread('CKSoln_solution_no_1.csv', 'C3..C3') %K
dist_1 = csvread('CKSoln_solution_no_1.csv', 'A2..A2') %cm
dist_2 = csvread('CKSoln_solution_no_1.csv', 'A3..A3') %cm

Z = ['Distance 1(cm):', num2str(dist_1)]
T = ['Temperature 1 (K):', num2str(Temp_1)]
W = ['Distance 2(cm):', num2str(dist_2)]
V = ['Temperature 2 (K):', num2str(Temp_2)]

%Set surface temperature to gas phase initial temperature from
%CHEMKIN output file
Ts = Temp_1

%Find heat flux to liquid from gas phase (for interface energy balance)
%Make sure units are ok in energy and mass calcs
dTdx = (Temp_2-Temp_1)/(dist_2-dist_1) %K/cm
dTdx = dTdx*100 %K/m
T_ave = (Temp_2+Temp_1)/2
[k] = Find_k (T_ave)
q_flux = k*dTdx %W/m^2

Y = ['Heat flux from gas phase (W/m^2):', num2str(q_flux)];
disp(Y)

%Added 12/7/15
%Calculate regression rate based on Ti, Ts, and heat of vaporization (Ts)
%call with necessary parameters to calculate condensed phase gasification
%i.e. Ts (or P, then find Ts for generality?), dTdx_plus
Ti = Temp_1
Tf = Temp_2
[rb] = Find_rb(dTdx, Ts, Ti, T_ave, Tf)

%**Compare calculated regression rate to assumed value (for gas phase input)
density_rho_chemkin = csvread('CKSoln_solution_no_1.csv', 'B2..B2') %g/cm^3
density_rho_chemkin = density_rho_chemkin/0.001 %kg/m^3 CHEMKIN writes out g/cm^3 and need to
change it
velocity_chemkin = csvread('CKSoln_solution_no_1.csv', 'D2..D2') %[cm/s]
velocity_chemkin = velocity_chemkin/100

```

```

density_htpb = 920 %kg/m^3
rb_assumed = (density_rho_chemkin*velocity_chemkin)/density_htpb %m/s

delta_rb = rb-rb_assumed %m/s

H = ['delta_rb (m/s):' num2str(delta_rb)]
disp('H')

%If not converged, create/update input file with new conditions
%look for better convergence routine (newton like)??
%keep history in an array?
%new_rb = rb_assumed+(rb_calc-rb_assumed)/2
%Chemkin takes awhile so to make things go faster:
%use a scaling factor
scaling_factor = 0.02

if (abs(delta_rb*scaling_factor)>0.00001)
    rb_new = rb_assumed+(scaling_factor*delta_rb)
else
    abs_delta = abs(delta_rb)
    new = (abs_delta/delta_rb)*0.00001
    rb_new = rb_assumed + new
endif
I = ['New rb guess is:',num2str(rb_new)]
disp(I)
%calculate new velocity off of new rb
velocity_new = (density_htpb*(rb_new))/(density_rho_chemkin) %m/s
velocity_new = velocity_new*100 %Change units to cm/s which chemkin is in

%Input file modify/write routines....
%Use the restart from previous run setting by adding RSTR keyword to input file
%rewrite old input file with loopcount suffix
%taken from http://www.mathworks.com/matlabcentral/answers/62986-how-to-change-a-specific-line-in-a-text-file
%http://www.mathworks.com/matlabcentral/answers/216298-how-to-change-a-specific-part-in-a-specific-line-in-a-text-file
% Read txt into line 88 where the fuel velocity will be changed

filename = 'OppDiff_HTPB_N2O22.inp';
newVal = velocity_new;
newValStr = num2str(newVal);

for i = length(newValStr)+1:-1:2
    newValStr(i) = newValStr(i-1);
end
newValStr(1) = ' ';
A = fileread(filename);
search = 'UINL Fuel_C1_Inlet1';
k = strfind(A, search);
k = k+length(search);
frontHalf = A(1:k);
k = k+1;

while A(k) ~= ' '
    k = k+1;
end

```

```

backHalf = A(k:end);
A = strcat(frontHalf, newValStr, backHalf)
fileID = fopen(filename, 'w');
fwrite(fileID, A);
fclose(fileID);

%Determine situation and write out final status/results

disp('convergence satisfied')
Pressure = csvread('CKSoln_solution_no_1_1.csv', 'C2..C2') %dyne/cm^2
Pressure = Pressure*0.1 %Convert dyne/cm^2 to pa 1dyne/cm^2 = 1Pa
Pressure2 = Pressure*1e-6 %convert to megapascals
P = ['Pressure (Pa):', num2str(Pressure)]
A = ['Pressure (MPa):', num2str(Pressure2)]
R = ['Regression rate:' num2str(rb_new)]
Z = ['Delta_Rb:' num2str(delta_rb)]
disp(P)
disp(A)
disp(R)
disp('see chemkin output for details')
disp('hit <enter> to end')

    loopcount= loopcount+1 %add this at the end so it actually iterates on the
                        %on the loopcount and doesn't do it before the
                        %actual for loop

```

endwhile

```

%Now to plot all the solutions!
%First obtain all the information and data using csvread
Temp = csvread('CKSoln_solution_no_1_1.csv', 'K2..K333'); %K
dist = csvread('CKSoln_solution_no_1_1.csv', 'A2..A333'); %cm
heat_release = csvread('CKSoln_solution_no_1_1.csv', 'B2..B333'); %erg/cm^3*sec
heat_release = heat_release*0.1; %convert to J/m^3*s
velocity = csvread('CKSoln_solution_no_1_1.csv', 'M2..M333'); %cm/sec

```

```

%mole fractions of species
CO = csvread('CKSoln_solution_no_1_1.csv', 'O2..O333');
CO2 = csvread('CKSoln_solution_no_1_1.csv', 'P2..P333');
NO = csvread('CKSoln_solution_no_1_1.csv', 'Q2..Q333');
H = csvread('CKSoln_solution_no_1_1.csv', 'S2..S333');
H2 = csvread('CKSoln_solution_no_1_1.csv', 'X2..X333');
O = csvread('CKSoln_solution_no_1_1.csv', 'T2..T333');
OH = csvread('CKSoln_solution_no_1_1.csv', 'U2..U333');
O2 = csvread('CKSoln_solution_no_1_1.csv', 'W2..W333');
H2O = csvread('CKSoln_solution_no_1_1.csv', 'Z2..Z333');
C = csvread('CKSoln_solution_no_1_1.csv', 'AH2..AH333');
C2H4 = csvread('CKSoln_solution_no_1_1.csv', 'AN2..AN333');
N = csvread('CKSoln_solution_no_1_1.csv', 'BL2..BL333');
N2O = csvread('CKSoln_solution_no_1_1.csv', 'BO2..BO333');
CN = csvread('CKSoln_solution_no_1_1.csv', 'BP2..BP333');

```

%Now plot results using plot

```

figure(1);
plot(dist,C2H4, dist,O2, dist, CO, dist, H2O, dist, H2, dist, CO2, dist, N2O, dist, NO);
title(['Mole fractions for ',num2str(Pressure2), 'MPa']);
xlabel('Distance (cm)');
ylabel('Mole Fractions ( )');
axis([0,0.5,0,1])
legend('C2H4','O2','CO','H2O','H2','CO2','N2O','NO');

```

```

figure(2);
plot(dist,Temp*1e6, dist, heat_release);
title(['Temperature and Heat Release Rate for ',num2str(Pressure2), 'MPa']);
xlabel('Distance (cm)');
ylabel('Temperature (K) and Heat Release Rate (erg/cm^3*sec)');
axis([0,0.5,-1e+10,2e+10])
legend('Temperature X 1E6', 'Heat Release Rate');

```

Subroutines to Follow:

```

## Author: PKN5018 <PKN5018@MNE-HPCL21>
## Created: 2015-12-04

```

```

function [delta_h] = Find_delta_sensible_enthalpy (Ti, Tf)
%Find sensible enthalpy difference in gas C2H4 between two temps by using
%finding integral of Cp dT of gas C2H4

```

```

MW = 28.05 %g/mol
MW2 = MW*1000 %g/kmol

```

```

%DIPPR Coefficients for ideal gas heat capacity
A = 3.338e4
B = 9.479e4
C = 1.596e3
D = 5.51e4
E = 7.408e2

```

```

%DIPPRR coefficients for liquid heat capacity
%A = 2.4739e560<
%B = -4.428e3
%C = 4.0936e1
%D = -1.697e-1
%E = 2.6816e-4

```

```

%DIPRR Cp values good for 60<T<1500 for ideal gas
if Ti>1500 %K
disp('Warning initial temperature for liquid sensible enthalpy (Cp_fit) out of range')
endif
if Tf>1500 %K
disp('Warning final temperature for liquid sensible enthalpy (Cp_fit) out of range')
endif

```

```

%DIPRR Cp values good for 104<T<252.7 for liquid
%if Ti>252.7 %K
%disp('Warning initial temperature for liquid sensible enthalpy (Cp_fit) out of range')
%endif
%if Tf>252.7 %K
%disp('Warning final temperature for liquid sensible enthalpy (Cp_fit) out of range')
%endif

```

```

%DIPRR Cp curve fit: Equation 100 for ideal gas
%A+B*[(C/T)/sinh(C/T)]^2+D*[(E/T)/cosh(E/T)]^2
%Integrate polynomial to get A*T + B*C*coth(C/T)-D*E*tanh(E/T) used wolframalpha to get integral
h_final = A*Tf+B*C*coth(C/Tf)-D*E*tanh(E/Tf)
h_initial = A*Ti+B*C*coth(C/Ti)-D*E*tanh(E/Ti)

%DIPRR Cp curve fit: Equation 100 for liquid
%A+(B*T) + (C*T^2)+(D*T^3)+(E*T^4)
%Integrate polynomial to get A*T+ 1/2(B*T^2) + (C/3)*T^3 + (D/4)*T^4 + (E/5)*T^5
%h_final = A*Tf+(B/2)*Tf^2+(C/3)*Tf^3+(D/4)*Tf^4+(E/5)*Tf^5
%h_initial = A*Ti+(B/2)*Ti^2+(C/3)*Ti^3+(D/4)*Ti^4+(E/5)*Ti^5

molar_delta_h = h_final-h_initial
%integrated DIPRR Cp yields J/kmol so convert to J/g
delta_h = (molar_delta_h/MW2) %J/g
U = ['delta_h', num2str(delta_h)]

Endfunction
function [qr] = Find_Heat_of_Reaction (Ts)
%Find heat of vapoization of liquid C2H4 at given surface temperaure in..
%Calculate liquid Cp for C2H4 as a function of T based on DIPRR fit

%C2H4 critical properties
MW = 28.05 %kg/kmol for C2H4
MW2 = 26.03728 %kg/kmol for C2H2
MW3 = (MW2+MW)/2
Tcrit = 282.34 %K http://encyclopedia.airliquide.com/encyclopedia.asp?GasID=29#MajorApplications

%DIPRR is down and cannot find coefficients so use Dr. Boyers for right now
%DIPRR values good for 102 to 282.34 K
%if Ts > 282.34
%disp('Warning: Temperature for heat of vaporization out of range')
%endif

%DIPRR coefficients
%A = 2.0639e7
%B = 8.0135e-1
%C = -8.128e-1
%D = 4.179e-1

%DIPRR says there is an E in the equation but not in the coefficients.....

%Calculate reduced temperature
%Tr = Ts/Tcrit
%DIPRR curve fit eqn 106
%e = B+C*Tr+D*Tr^2
%molar_Lvap = A*(1-Tr)^e %J/kmol
%DIPRR proerty given in J/KMOL, so divide by molecular weight of C2H4 and
%convert to J/g to get in energy/mass units
%Lvap = (molar_Lvap/MW)/1000 %J/g

%L = ['Lvap:', num2str(Lvap)]
%disp(L)

%Determine Heat of Reaction since it goes from solid to gas due to qr

```

```

%C7.337+H10.982 <--> XC2H4+j*C2H2
%Do a stiochiometric eqn and solve it
x = 1.83425
j = 1.83425    %Added C2H2 instead to conserve C

%Now that the stiochiometric coefficients are solved for solve for the qr
%qr = Hproducts-Hreactants
%Products at Ts of 600K may have to change depending on the temperature you need
deltaH_C2H2 = 15.771 %KJ/mol
Hf_C2H2 = 216.993 %KJ/mol

deltaH_C2H4 = 17.335 %KJ/mol
Hf_C2H4 = 44.294 %KJ/mol

%deltaH_O2 = 9.244 %KJ/mol
%deltaH_N2 = 8.894 %KJ/mol

%Hf_CO = 8.942 %added in to see if it changed anything based upon a non balance of values for HTPB to C2H4
%deltaH_CO = -110.15 %added in to see if it changed anything

%Reactants at Tr of 298K
%Hf_N2O = 82.05 %KJ/mol http://webbook.nist.gov/cgi/cbook.cgi?ID=C10024972&Mask=1
Hf_HTPB = -51.8 %KJ/mol http://www.lr.tudelft.nl/en/organisation/departments/space-engineering/space-systems-engineering/expertise-areas/space-propulsion/design-of-elements/rocket-propellants/solids/physical-properties/

Hproducts = (x*(deltaH_C2H4+Hf_C2H4)+j*(deltaH_C2H2+Hf_C2H2))
Hreactants = Hf_HTPB
qr_molar = Hproducts-Hreactants %in KJ/mol

MW_HTPB = 138 %g/mol
%Should I use MW_HTPB or MW of C2H4??
qr = (qr_molar/MW_HTPB)*1000 %J/g

Q = ['Heat of reaction: J/g', num2str(qr)]
disp(Q)

%heat of formation for HTPB and N2O is in the Rocket Propulsion elements book on page 583!!!!!!
Endfunction
function [k] = Find_k (T_ave)
%Find thermal conductivity of gas at given temperature in W/m-K
%DIPPR coefficients from http://dippr.byu.edu/public/chemsearch.asp?Mode=Printout2&ChemID=201
%DIPPR coefficients for C2H4 right now since that is the gaseous fuel
%A = 8.6806e-6
%B = 1.4559
%C = 2.9972E2
%D = -2.9403e4

%for testing, use an approximate constant value ***fixme***
%k = 2e-2 %W/m-K

%Once working calculate k for C2H4 as a function of T based on DIPPR fit
%DIPPR values good for 170K to 590K
%if T_ave>590
%disp('Warning temperature for thermal conductivity (k) fit out of range')
%endif

```

```
%DIPRR curve fit: http://dippr.byu.edu/public/calculator.asp?ChemID=201&PropertyID=VTC&SetOrder=A
%k = (A*T_ave^B)/((1+(C/T_ave)+(D/T_ave^2))) %W/m*K
%DIPRR properties in W/m*K
```

```
f1 = csvread('CKSoln_solution_no_1.csv', 'E2..E2') %Erg/cm*K*s
f2 = csvread('CKSoln_solution_no_1.csv', 'E3..E3') %Erg/cm*K*s
f = (f1+f2)/2
k = f*1E-7 %W/m*K
K = ['thermal conductivity K=(W/m*K)', num2str(k)]
disp(K)
```

```
endfunction
```

```
function [rb] = Find_rb (dTdx, Ts, Ti, T_ave, Tf)
[k] = Find_k (T_ave)
[qr] = Find_Heat_of_Reaction (Ts)
[rho_gas] = Find_rho_gas(Ti)
[delta_h] = Find_delta_sensible_enthalpy(Ti,Tf)
```

```
q = k*dTdx %J/s*m^2
```

```
%Find Evaporation flux based on heat flux (vaporization)
m_flux_gassification = q/(delta_h-qr) %Check units g/s*m^2
```

```
%for CHEMKIN, need mass flux in g/cm^2*s
%check units on preproperty lookup subroutines
%---> use modot times desnity (DIPPR lookup at initial
rb = abs(m_flux_gassification/rho_gas) %Check units should be m/s
```

```
endfunction
```

```
function [rho_gas] = Find_rho_gas (Ts)
%Find density of liquid of C2H4 at given surface temperature in g/cm^3
MW = 28.05 %g/mol for C2H4
MW2 = 26.04 %g/mol for C2H2
MW3 = (MW+MW2)/2
```

```
%calculate liquid density for C2H4 as a function of T based on DIPRR fit
%DIPRR coefficients
%A = 2.0961
%B = 2.7657e-1
%C = 2.8234e2
%D = 2.9147e-1
```

```
%Temperature range for eqn 104K<T<282.34K
%Liquid density DIPRR eqn from eqn 105
%e2 = 1+(1-Ts/C)^D
%rho_liquid = A/ (B^e2)
```

```
%for testing, use an approximate constant value
Pressure = csvread('CKSoln_solution_no_1_1.csv', 'C2..C2') %dyne/cm^2
Pressure = Pressure*0.1 %Convert dyne/cm^2 to pa 1dyne/cm^2 = 1Pa
Ru = 8314 %J/kmol*K
R = Ru/MW3 %J/kg*K
rho_gas = Pressure/(R*Ts) %kg/m^3
rho_gas = rho_gas*1000 %g/m^3
```

%Find rho_gas based upon Ideal Gas Law

Endfunction

function [N, R, Q, F] = Set_CHEMKIN_env ()

% Establish the CHEMKIN environment (see section 4.1.2 in "Getting Started")

% Open a DOS window and type set in the DOS window

% Use setenv to set environment values and getenv retrieves the value specified in

% the setenv

%Set REACTION_DIR = C:\Program Files\Reaction

%Set CHEMKIN_VERS=10141

%Set CHEMKIN_BIN = C:\Program Files\Reaction\chemkin15141_win64\bin

%Set CHEMKIN_RELEASE_NUMBER = 10141 <x64> (08 Jul 2015)

%Set shell environment variables

setenv('REACTION_DIR','C:\Program Files\Reaction');

N = getenv('REACTION_DIR');

setenv('CHEMKIN_VERS=15151');

R = getenv('CHEMKIN_VERS');

setenv('CHEMKIN_BIN','C:\Program Files\Reaction\chemkin15151_win64\bin');

Q = getenv('CHEMKIN_BIN');

setenv('CHEMKIN_RELEASE_NUMBER=Release_15151 <x64> (18 Jan 2016)');

F = getenv('CHEMKIN_RELEASE_NUMBER');

%Set PATH to include CHEMKIN binary directory

S = 'CHEMKIN environment set.'

disp(S)

endfunction

function [cmdout4] = Run_shell (shell_cmd)

[shell_result, cmdout4] = system(shell_cmd)

%if (shell_result==1)

 %shell_err = ierrno()

 %disp('Error')

 %disp('Error trying to execute the following shell command.')

%endif

endfunction

Appendix G: Transport Input Data

```

!*****BEGIN-HDR
!
! Copyright (c) 1997-2006 Reaction Design. All rights reserved.
!
! $Header: /chemkin/4.2/prebuild/data/tran.dat 8      12/21/06 9:20a Frupley $
!
! $NoKeywords: $
!*****END-HDR
AR          0    136.500    3.330    0.000    0.000    0.000
AR*         0    136.500    3.330    0.000    0.000    0.000
C           0     71.400    3.298    0.000    0.000    0.000  ! (*)
C2          1     97.530    3.621    0.000    1.760    4.000
C2O         1    232.400    3.828    0.000    0.000    1.000  ! *
CN2         1    232.400    3.828    0.000    0.000    1.000  ! OIS
C2H         1    209.000    4.100    0.000    0.000    2.500
C2H2        1    209.000    4.100    0.000    0.000    2.500
C2H2OH      2    224.700    4.162    0.000    0.000    1.000  ! (*)
CH2OH       2    417.000    3.690    1.700    0.000    2.000
C2H3        2    209.000    4.100    0.000    0.000    1.000  ! (*)
C2H4        2    280.800    3.971    0.000    0.000    1.500
C2H5        2    252.300    4.302    0.000    0.000    1.500
C2H6        2    252.300    4.302    0.000    0.000    1.500
C2N         1    232.400    3.828    0.000    0.000    1.000  ! OIS
C2N2        1    349.000    4.361    0.000    0.000    1.000  ! (OIS)
C3H2        2    209.000    4.100    0.000    0.000    1.000  ! (*)
C3H3        1    252.000    4.760    0.000    0.000    1.000
C3H4        1    252.000    4.760    0.000    0.000    1.000
C3H4P       1    252.000    4.760    0.000    0.000    1.000  ! JAM
C3H6        2    266.800    4.982    0.000    0.000    1.000
C3H7        2    266.800    4.982    0.000    0.000    1.000
C4H6        2    357.000    5.180    0.000    0.000    1.000
I*C3H7      2    266.800    4.982    0.000    0.000    1.000
N*C3H7      2    266.800    4.982    0.000    0.000    1.000
C3H8        2    266.800    4.982    0.000    0.000    1.000
C4H         1    357.000    5.180    0.000    0.000    1.000
C4H2        1    357.000    5.180    0.000    0.000    1.000
C4H2OH      2    224.700    4.162    0.000    0.000    1.000  ! (*)
C4H3        1    357.000    5.180    0.000    0.000    1.000
C4H4        1    357.000    5.180    0.000    0.000    1.000
C4H8        2    357.000    5.176    0.000    0.000    1.000
C4H9        2    357.000    5.176    0.000    0.000    1.000
S*C4H9      2    357.000    5.176    0.000    0.000    1.000
C4H9        2    357.000    5.176    0.000    0.000    1.000
I*C4H9      2    357.000    5.176    0.000    0.000    1.000
C5H2        1    357.000    5.180    0.000    0.000    1.000
C5H3        1    357.000    5.180    0.000    0.000    1.000
C6H2        1    357.000    5.180    0.000    0.000    1.000
C6H5        2    412.300    5.349    0.000    0.000    1.000  ! JAM
C6H5 (L)    2    412.300    5.349    0.000    0.000    1.000  ! JAM
C6H5O       2    450.000    5.500    0.000    0.000    1.000  ! JAM
C5H5OH      2    450.000    5.500    0.000    0.000    1.000  ! JAM
C6H6        2    412.300    5.349    0.000    0.000    1.000  ! SVE
C6H7        2    412.300    5.349    0.000    0.000    1.000  ! JAM
CH          1     80.000    2.750    0.000    0.000    0.000
CH2         1    144.000    3.800    0.000    0.000    0.000
CH2 (S)     1    144.000    3.800    0.000    0.000    0.000
CH2 (SING)  1    144.000    3.800    0.000    0.000    0.000
CH2CHCCH    2    357.000    5.180    0.000    0.000    1.000  ! JAM
CH2CHCCH2   2    357.000    5.180    0.000    0.000    1.000  ! JAM
CH2CHCH2    2    260.000    4.850    0.000    0.000    1.000  ! JAM

```

CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000 ! JAM
CH2CHCHCH2	2	357.000	5.180	0.000	0.000	1.000 ! JAM
CH2CO	2	436.000	3.970	0.000	0.000	2.000
CH2O	2	498.000	3.590	0.000	0.000	2.000
CH3	1	144.000	3.800	0.000	0.000	0.000
CH3CC	2	252.000	4.760	0.000	0.000	1.000 ! JAM
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000 ! JAM
CH3CCCH3	2	357.000	5.180	0.000	0.000	1.000 ! JAM
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000 ! JAM
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000 ! JAM
CH3CH2CCH	2	357.000	5.180	0.000	0.000	1.000 ! JAM
CH3CHO	2	436.000	3.970	0.000	0.000	2.000
CH3CO	2	436.000	3.970	0.000	0.000	2.000
CH3O	2	417.000	3.690	1.700	0.000	2.000
CH3OH	2	481.800	3.626	0.000	0.000	1.000 ! SVE
CH3HCO	2	436.000	3.970	0.000	0.000	2.000 ! Added myself for
transport data needed for program						
OCHCHO	2	406.937	4.823	0.000	0.000	2.000 ! Added myself for
transport data needed for program						
C2H5CHO	2	435.200	4.662	2.700	0.000	1.000 ! Added myself for
transport data needed for program						
C2H5CO	2	424.600	4.820	0.000	0.000	1.000 ! Added myself for
transport data needed for program						
NO3	2	200.000	3.500	0.000	0.000	1.000 ! Added myself for
transport data needed for program						
HONO	2	232.400	3.828	0.000	0.000	1.000 ! Added myself for
transport data needed for program						
CH3CN	2	436.000	3.970	0.000	0.000	2.000 ! Added myself for
transport data needed for program						
CH2CN	2	436.000	3.970	0.000	0.000	2.000 ! Added myself for
transport data needed for program						
CH4	2	141.400	3.746	0.000	2.600	13.000
CH4O	2	417.000	3.690	1.700	0.000	2.000
CN	1	75.000	3.856	0.000	0.000	1.000 ! (OIS)
CNC	1	232.400	3.828	0.000	0.000	1.000 ! OIS
CNN	1	232.400	3.828	0.000	0.000	1.000 ! OIS
CO	1	98.100	3.650	0.000	1.950	1.800
CO2	1	244.000	3.763	0.000	2.650	2.100
CL	0	130.8	3.613	0.000	0.000	1.000 ! (singh)
CL-	0	130.8	3.613	0.000	0.000	1.000 ! (singh)
E	0	850.	425.	0.000	0.000	1.000 ! (singh)
F	0	80.000	2.750	0.000	0.000	0.000
F2	1	125.700	3.301	0.000	1.600	3.800
H	0	145.000	2.050	0.000	0.000	0.000
H2C4O	2	357.000	5.180	0.000	0.000	1.000 ! JAM
H2	1	38.000	2.920	0.000	0.790	280.000
H2CCCCH	2	357.000	5.180	0.000	0.000	1.000 ! JAM
H2CCCCH2	2	357.000	5.180	0.000	0.000	1.000 ! JAM
H2CCCH	2	252.000	4.760	0.000	0.000	1.000 ! JAM
H2CN	1	569.000	3.630	0.000	0.000	1.000 ! os/jm
H2NO	2	116.700	3.492	0.000	0.000	1.000 ! JAM
H2O	2	572.400	2.605	1.844	0.000	4.000
H2O2	2	107.400	3.458	0.000	0.000	3.800
H2S	2	301.000	3.600	0.000	0.000	1.000 ! (OIS)
HC2N2	1	349.000	4.361	0.000	0.000	1.000 ! OIS
HCCHCCH	2	357.000	5.180	0.000	0.000	1.000 ! JAM
HCCO	2	150.000	2.500	0.000	0.000	1.000 ! (*)
HCCOH	2	436.000	3.970	0.000	0.000	2.000
HCN	1	569.000	3.630	0.000	0.000	1.000 ! (OIS)
HCNO	2	232.400	3.828	0.000	0.000	1.000 ! JAM
HCO	2	498.000	3.590	0.000	0.000	0.000
HCO+	1	498.000	3.590	0.000	0.000	0.000
HCL	1	344.7	3.339	0.000	0.000	1.000 ! (singh)

HF	1	330.000	3.148	1.920	2.460	1.000	! sv/mec
HF0	1	352.000	2.490	1.730	0.000	5.000	
HF1	1	352.000	2.490	1.730	0.000	5.000	
HF2	1	352.000	2.490	1.730	0.000	5.000	
HF3	1	352.000	2.490	1.730	0.000	5.000	
HF4	1	352.000	2.490	1.730	0.000	5.000	
HF5	1	352.000	2.490	1.730	0.000	5.000	
HF6	1	352.000	2.490	1.730	0.000	5.000	
HF7	1	352.000	2.490	1.730	0.000	5.000	
HF8	1	352.000	2.490	1.730	0.000	5.000	
CH2HCO	2	436.000	3.970	0.000	0.000	2.000	
HOCN	2	232.400	3.828	0.000	0.000	1.000	! (JAM)
HNCO	2	232.400	3.828	0.000	0.000	1.000	! (OIS)
HNNO	2	232.400	3.828	0.000	0.000	1.000	! (*)
HNO	2	116.700	3.492	0.000	0.000	1.000	! (*)
HNOH	2	116.700	3.492	0.000	0.000	1.000	! JAM
HO2	2	107.400	3.458	0.000	0.000	1.000	! (*)
HSO2	2	252.000	4.290	0.000	0.000	1.000	! (OIS)
HE	0	10.200	2.576	0.000	0.000	0.000	! (*)
K	0	850.	4.25	0.000	0.000	1.000	! (singh)
KCL	1	1989.	4.186	0.000	0.000	1.000	! (singh)
KO	1	383.0	3.812	0.000	0.000	1.000	! (singh)
KOH	2	1213.	4.52	0.000	0.000	1.000	! (singh)
KO2	2	1213.	4.69	0.000	0.000	1.000	! (singh)
KH	1	93.3	3.542	0.000	0.000	1.000	! (singh)
K+	0	850.	4.25	0.000	0.000	1.000	! (singh)
N	0	71.400	3.298	0.000	0.000	0.000	! (*)
N2	1	97.530	3.621	0.000	1.760	4.000	
N2H2	2	71.400	3.798	0.000	0.000	1.000	! (*)
N2H3	2	200.000	3.900	0.000	0.000	1.000	! (*)
N2H4	2	205.000	4.230	0.000	4.260	1.500	
N2O	1	232.400	3.828	0.000	0.000	1.000	! (*)
NCN	1	232.400	3.828	0.000	0.000	1.000	! OIS
NCO	1	232.400	3.828	0.000	0.000	1.000	! (OIS)
NH	1	80.000	2.650	0.000	0.000	4.000	
NH2	2	80.000	2.650	0.000	2.260	4.000	
NH3	2	481.000	2.920	1.470	0.000	10.000	
NNH	2	71.400	3.798	0.000	0.000	1.000	! (*)
NO	1	97.530	3.621	0.000	1.760	4.000	
NCNO	2	232.400	3.828	0.000	0.000	1.000	! OIS
NO2	2	200.000	3.500	0.000	0.000	1.000	! (*)
O	0	80.000	2.750	0.000	0.000	0.000	
O2	1	107.400	3.458	0.000	1.600	3.800	
O3	2	180.000	4.100	0.000	0.000	2.000	
OH	1	80.000	2.750	0.000	0.000	0.000	
S	0	847.000	3.839	0.000	0.000	0.000	! (OIS)
S2	1	847.000	3.900	0.000	0.000	1.000	! (OIS)
SH	1	847.000	3.900	0.000	0.000	1.000	! (OIS)
SO	1	301.000	3.993	0.000	0.000	1.000	! (OIS)
SO2	2	252.000	4.290	0.000	0.000	1.000	! (OIS)
SO3	2	378.400	4.175	0.000	0.000	1.000	! (OIS)
!							
! Local Additions for Silicon CVD							
!							
H2SISIH2	2	312.6	4.601	0.000	0.000	1.000	! (mec)
H3SISIH	2	312.6	4.601	0.000	0.000	1.000	! (mec)
SI	0	3036.	2.910	0.000	0.000	0.000	! (mec)
SIH	1	95.8	3.662	0.000	0.000	1.000	! (mec)
SIH2	2	133.1	3.803	0.000	0.000	1.000	! (mec)
SIH2 (3)	2	133.1	3.803	0.000	0.000	1.000	! (mec)
SIH3	2	170.3	3.943	0.000	0.000	1.000	! (mec)
SIH4	2	207.6	4.084	0.000	0.000	1.000	! (mec)
SI2	1	3036.	3.280	0.000	0.000	1.000	! (mec)

SI2H2	2	323.8	4.383	0.000	0.000	1.000	! (mec)
SI2H3	2	318.2	4.494	0.000	0.000	1.000	! (mec)
SI2H4	2	312.6	4.601	0.000	0.000	1.000	! (mec)
SI2H5	2	306.9	4.717	0.000	0.000	1.000	! (mec)
SI2H6	2	301.3	4.828	0.000	0.000	1.000	! (mec)
SI3	2	3036.	3.550	0.000	0.000	1.000	! (mec)
SI3H8	2	331.2	5.562	0.000	0.000	1.000	! (mec)
C-SI3H6	2	331.2	5.562	0.000	0.000	1.000	! (mec)
SIH3SIH2SIH	2	331.2	5.562	0.000	0.000	1.000	! (mec)
!							
! Local Additions for GaAs MOCVD							
!							
AS	0	1045.5	4.580	0.000	0.000	0.000	! (mec)
ASH	1	199.3	4.215	0.000	0.000	1.000	! (mec)
ASH2	2	229.6	4.180	0.000	0.000	1.000	! (mec)
ASH3	2	259.8	4.145	0.000	0.000	1.000	! (mec)
Ash3	2	259.8	4.145	0.000	0.000	1.000	
! (Reid et al.)							
AS2	1	1045.5	5.510	0.000	0.000	1.000	! (mec)
GA	0	2961.8	4.62	0.000	0.000	0.000	! (mec)
GAH	1	335.5	4.24	0.000	0.000	1.000	! (mec)
GAME	2	972.7	4.92	0.000	0.000	1.000	! (mec)
GAME2	2	675.8	5.22	0.000	0.000	1.000	! (mec)
GAME3	2	378.2	5.52	0.000	0.000	1.000	! (mec)
GaMe3	2	378.2	5.52	0.000	0.000	1.000	! (mec)
TMG	2	378.2	5.52	0.000	0.000	1.000	! (mec)
DMG	2	675.8	5.22	0.000	0.000	1.000	! (mec)
GACH3	2	972.7	4.92	0.000	0.000	1.000	! (mec)
H2ASCH3	2	408.0	4.73	0.000	0.000	1.000	! (mec)
Al2Me6	2	471.	6.71	0.0	0.0	1.0	! hkm 11/94
AlMe3	2	471.	5.30	0.0	0.0	1.0	! hkm 11/94
!							
! Local Additions for Silicon Nitride CVD							
!							
SIF	1	585.0	3.318	0.000	0.000	1.000	! (sve)
SIF3	2	309.6	4.359	0.000	0.000	1.000	! (mec)
SIF3NH2	2	231.0	4.975	0.000	0.000	1.000	! (mec)
SIF4	2	171.9	4.880	0.000	0.000	1.000	! (sve)
SIHF3	2	180.8	4.681	0.000	0.000	1.000	! (mec)
!							
! Local Additions for SiO2 CVD							
!							
C2H5OH	2	362.6	4.53	0.000	0.000	1.000	! (sve)
OSI (OC2H5) 2	2	522.7	7.03	0.000	0.000	1.000	! (mec)
Si (OC2H5) 4	2	522.7	7.03	0.000	0.000	1.000	! (mec)
Si (OH) (OC2H5) 3	2	522.7	7.03	0.000	0.000	1.000	! (noest)
SI (OC2H5) 4	2	522.7	7.03	0.000	0.000	1.000	! (mec)
SI (OH) (OC2H5) 3	2	522.7	7.03	0.000	0.000	1.000	! (noest)
SI (OH) 2 (OC2H5) 2	2	522.7	6.35	0.000	0.000	1.000	! (noest)
Si (OH) 2 (OC2H5) 2	2	522.7	6.35	0.000	0.000	1.000	! (noest)
SI (OH) 3 (OC2H5)	2	522.7	5.75	0.000	0.000	1.000	! (noest)
SI (OH) 4	2	522.7	5.25	0.000	0.000	1.000	! (noest)
O (Si (OC2H5) 3) 2	2	522.7	5.25	0.000	0.000	1.000	! (noest)
O (SI (OC2H5) 3) 2	2	522.7	5.25	0.000	0.000	1.000	! (noest)
!							
! Local Additions for Halogen Diamonds							
!							
CF	1	94.2	3.635	0.000	0.000	1.000	! (sve)
CF2	2	108.0	3.977	0.000	0.000	1.000	! (sve)
CF3	2	121.0	4.320	0.000	0.000	1.000	! (sve)
CHF3	2	240.0	4.330	0.000	0.000	1.000	! (sve)
CF4	2	134.0	4.662	0.000	0.000	1.000	! (sve)
CH2F2	2	318.0	4.080	0.000	0.000	1.000	! (sve)

C2F4	2	202.6	5.164	0.000	0.000	1.000	!(mec)
C2F6	2	194.5	5.512	0.000	0.000	1.000	!(mec)
! New entries for In, InMe3, PH3, InAsMe							
PH3	2	251.5	3.981	0.000	0.000	1.000	
!(Reid et al.)							
BCL3	2	337.7	5.127	0.000	0.000	1.000	!svehla
CL2BNH2	2	337.7	5.127	0.000	0.000	1.000	
!mec guess							

Appendix H: Calibrations

Pressure Transducer

The pressure transducers that were used in the motor and opposed flow burner studies were Setra Model 206 (Industrial Pressure Transducer) transducers. These were chosen based upon the high performance, reliability, versatility and ability to record 1000 Hz for a longer time span. The pressure ranges of the transducers used was 0-1000 psig to 0-3000 psig. To calibrate the transducer, a gauge calibration box was used. Inert gas was supplied to the gauge box with the pressure transducer connected to it as well. An excitation voltage was supplied while a BNC cable obtained the voltage output of the transducer. Pressure was supplied with increments of 50 psig up to a level given the range of the Setra. Afterwards a linear fit was applied to get an equation correlating voltage to a given pressure.

Choked Flow of Fuel and Ideal Gas

When conducting experiments with the opposed flow burner using N_2O oxidizer, the apparatus enters supercritical conditions. Unfortunately these conditions that were seen when using the counterflow burner are above the critical temperature and most likely pressure, where N_2O begins to deviate from the ideal gas law (becoming non-linear with the dependence of density on pressure). Therefore, the choked flow equations used to obtain a mass flow rate can no longer be used, so an empirical equation was generated as a function of upstream pressure and orifice diameter. This was accomplished by recording the upstream pressure and mass flow rate downstream with a bubble meter. This was done for two different orifice sizes, generating a polynomial fit to the normalized flow rate. A polynomial was then generated for mass flow rate as a function of upstream pressure for each orifice. The results are shown in Figure H.1 and the empirical equation provided in Eq. H.1.

$$\dot{m} = 17.98P^2 + 276.17P + 16.188 \quad (\text{H.1})$$

where the mass flow is in g/s and P is in MPa.

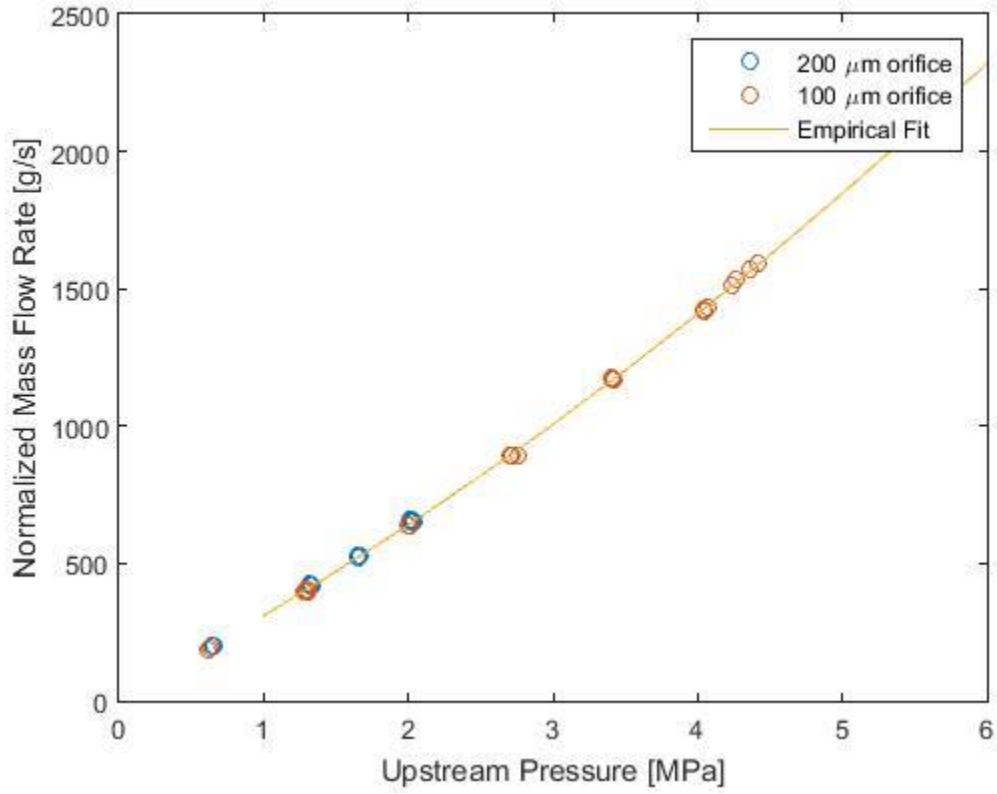


Figure H.1: Empirical fits for normalized N₂O mass flow rates.