A COMPUTATIONAL STUDY OF THE IGNITION OF
PREMIXED METHANE AND OXYGEN VIA A HOT STREAM

by

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Dedication:

I would like to dedicate this work to my family, those who are with me now, those who have passed, and all of our ever growing family. Being away and challenging myself to new tasks have made me realize how much your support throughout my life has helped shape me into who I am and bring me to where I am. I'm truly grateful for everything; I have no doubt that I would not have been able to do this without you.

I hope I've made you proud.

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List of Abbreviations

A – cross sectional area – m^2

a – strain rate – $\frac{1}{s}$

a_i – internal surface area per unit length – m^2

a_e – surface area of section with heat flux per unit length – m^2

$\dot{b}_k$ – molar production rate of bulk solid k^{th} species by surface reactions – $\frac{\text{moles}}{m^2 * s}$

$\bar{C}_p$ – mean heat capacity per unit mass of the gas – $\frac{\text{ergs}}{\text{kg} * K}$

c_p – specific heat of the mixture – $\frac{\text{ergs}}{\text{kg} * K}$

$c_{p,k}$ – specific heat of the k^{th} species – $\frac{\text{ergs}}{\text{kg} * K}$

F – drag force exerted on the gas by the tube wall – Newtons

f' – function related to derivative of modified stream function (see text)

$\dot{g}_k$ – molar production rate of k^{th} species by all surface reactions – $\frac{\text{moles}}{m^2 * s}$

h_k – specific enthalpy of k^{th} species – $\frac{\text{ergs}}{\text{kg}}$

K – total number of species – #

K_b – total number of bulk solid species – #

K_g – total number of gas phase species – #

k – representative species number – #

λ – thermal conductivity $\frac{\text{erg}}{m * K * s}$

$$\mu - \text{viscosity} - \frac{\text{kg}}{\text{m} * \text{s}}$$

$$P - \text{pressure} - \text{atm}$$

$$P_{\text{in}} - \text{tube inlet pressure} - \text{atm}$$

$$\phi - \text{equivalence ratio}$$

$$Q_e - \text{heat flux of tube wall} - \frac{\text{ergs}}{\text{m}^2 * \text{s}}$$

$$Q_i - \text{heat flux to the mixture from inner tube wall} - \frac{\text{ergs}}{\text{m}^2 * \text{s}}$$

$$Q_{i,\text{assigned}} - \text{assigned heat flux magnitude at given } i^{\text{th}} \text{ location} - \frac{\text{ergs}}{\text{m}^2 * \text{s}}$$

$$R - \text{universal gas constant} - \frac{\text{ergs}}{\text{K} * \text{mole}}$$

$$\rho - \text{density} - \frac{\text{kg}}{\text{m}^3}$$

$$\rho_e - \text{density at entrance} - \frac{\text{kg}}{\text{m}^3}$$

$$\rho_F - \text{density at premixed fuel/oxidizer side boundary} - \frac{\text{kg}}{\text{m}^3}$$

$$\rho_I - \text{density at igniter side boundary} - \frac{\text{kg}}{\text{m}^3}$$

$$\dot{s}_k - \text{production rate of } k^{\text{th}} \text{ surface species} - \frac{\text{moles}}{\text{m}^2 * \text{s}}$$

$$T - \text{temperature} - \text{Kelvin}$$

$$T_F - \text{temperature of mixture at premixed side boundary} - \text{Kelvin}$$

$$T_I - \text{temperature of incoming stream at igniter side boundary} - \text{Kelvin}$$

$$t - \text{time} - \text{seconds}$$

$$u - \text{axial velocity} - \frac{\text{m}}{\text{s}}$$

u_{in} – tube inlet axial velocity – $\frac{m}{s}$

u_e – axial velocity at entrance – $\frac{m}{s}$

V – axial component of the mass flux – $\frac{kg}{m^2 * s}$

V_{ky} – diffusion velocity in the axial direction of the k^{th} species – $\frac{m}{s}$

V_F – axial component of the mass flux at premixed side boundary – $\frac{kg}{m^2 * s}$

V_I – axial component of the mass flux at igniter side boundary – $\frac{kg}{m^2 * s}$

v – velocity in axial direction – $\frac{m}{s}$

$\bar{W}$ – average molecular weight – kg

W_k – molecular weight of k^{th} species – kg

ω_k – molar production rate of k^{th} species by homogenous gas reactions – $\frac{moles}{m^3 * s}$

x_k – mole fraction of k^{th} species

x – axial distance in tube – m

y – axial distance in counterflow – m

Y_k – mass fraction of k^{th} species

$Y_{k,F}$ – mass fraction of k^{th} species at premixed fuel side boundary

$Y_{k,I}$ – mass fraction of k^{th} species at igniter side boundary

$Y_{k,in}$ – mass fraction of k^{th} species at tube inlet boundary

Z_k – site fractions of k^{th} species

A Computational Study of the Ignition of Premixed Methane and Oxygen via a Hot Stream

Abstract

by

MATTHEW CHARLES DEANS

With methane being a fuel to be utilized in the future of space exploration, alternative ignition systems need to be developed. This study computationally focuses on the ignition of methane and oxygen mixtures in a counterflow configuration by a heated stream. Most combustion systems have non-uniform and/or non-homogenous flow, species, and temperature fields. This configuration allows for the study of both chemical kinetics as well as convective-diffusive transport effects. The effects of strain rate, pressure, and equivalence ratio on ignition are examined. A catalytic simulation code is used to generate ranges of combustion product composition and temperature when using a catalytic reactor for the hot stream. The vitiation of these into the hot stream is conducted to determine their influence on ignition. Tests with the individual components in a range up to the maximum possible achievable level will be carried out to determine the separate effects. A combined case simulating the potential of an actual catalytic igniter is also run to confirm the feasibility of such a technology and the combined effects of the different species.

Chapter 1: Introduction

1.1: Background

New concerns and goals in the development of combustion systems, from fuel efficiency and availability to the exploration of a planet no person has set foot on before, have provided the chance to utilize fuels that may not have been used for a given purpose before. With the initial development of the Space Shuttle program in the late 1960's and early 1970's, the choice had been made to propel the craft with liquid hydrogen as a fuel, accompanied by solid rocket boosters. With the creation of the Orion, the new crew exploration vehicle that will replace the space shuttles, various fuels are to be used. With the eventual goal being manned missions to Mars, the potential exists to utilize methane as a fuel given that, as part of in-situ resource utilization (ISRU), it can be produced on Mars. This would thus eliminate the need, and the accompanying extra weight, of carrying the fuel to return home. In fact, the CEV crew module is being designed with thrusters utilizing oxygen and methane (Hatfield, 2006).

Methane as a fuel has many beneficial properties, including those that are chemical, thermodynamic, and fluidic, which can be taken advantage of (Colket *et al.*, 2001, Pempie *et al.*, 2001, Burkhardt *et al.*, 2002). Because of these advantages and the growing importance of the ISRU factor, methane may be the fuel of choice for this venture if the proper systems can be developed and if a few concerns can be addressed. If optimized for the longer ignition times of methane and in combination with combustion assisting techniques such as the cracking of the fuel, standard ignition systems, such as an augmented spark ignition, can be used to sustain combustion but with the wholly new

development of the craft, it gives an opportunity to use this as a redundant system that might be more advantageous for a given situation (Armstrong, 1989).

A catalytic ignition system has the advantages of requiring lower temperature and potentially less energy to induce a reaction than other direct delivery methods. In comparison with a spark system, a catalytic system may require less power and have a lower voltage requirement. Larger voltages result in larger and heavier power sources. Even in comparison with an automobile spark plug, which would require on the order of 10 kV and 50 Watts, initial estimates for a catalytic system would require less than a fifth of this power and a low voltage as the energy is delivered in a heating process. As a redundant system, the power system already used for the primary system would be more than able to provide what would be required for this backup. The very nature of catalysts allows for not only the achievement of higher temperatures, but control of magnitude based on initial temperature, residence time, and initial mixture composition. Different catalysts may cause different effects but platinum, which is used for this study, is efficient at initiating reactions with hydrogen and hydrocarbons (Deutschmann *et al.*, 1996, Boyarko *et al.*, 2005, Volchko *et al.*, 2006, Mento *et al.*, 2006). Additionally, it is a system that does not just yield un-reacted fuel/oxidizer or fully reacted products but allows for control over which radicals may be present at the end of the catalytic reactor, potentially aiding ignition. This study should allow some understanding and potential use of such technology in space exploration.

1.2: Approach

While research has been carried out examining ignition in non-premixed counterflowing methane versus heated air, (Fotache *et al.*, 1997) the investigations on

ignition of methane/oxygen, in both non-premixed and premixed modes, are meager. Therefore, this study will venture into this realm of ignition, with special emphasis on premixed condition and elevated pressures. Specifically, ignition of a premixed methane/oxygen jet by a heated counterflow is computationally investigated with detailed chemistry and thermodynamic/transport properties, at varying equivalence ratios and pressures. For the sake of these trials, the equivalence ratio will be defined as the following.

$$\phi = \frac{\frac{X_{Fuel}}{X_{Oxidizer}}}{\frac{X_{Fuel \text{ at Stoichiometric}}}{X_{Oxidizer \text{ at Stoichiometric}}}}$$

It is noted that in most practical situations the species and temperature fields are inhomogeneous while the flow is non-uniform. Thus, effects of convective-diffusive transport on the ignition process need to be characterized, in addition to chemical kinetics.

Furthermore, the effects of chemical vitiation in the hot stream on ignition limits will be also examined. This is of interest as methane is typically a slower reacting fuel, requiring higher ignition temperature. The feasibility of promoting ignition through vitiated species in the heated counterflow will be explored. The baseline operation of ignition by heated nitrogen will be fully studied as will the vitiation effects of the combustion products. Through the comparison, the benefits of using these products through some system such as a catalytic igniter will be assessed.

1.3: Configuration

In order to study the effects of the variation conducted in this study, they can be canonically simulated by the counterflow configuration. With this counterflow

configuration, the effects of equivalence ratio, aerodynamic straining, and pressure on counterflow ignition limits will be systematically studied. As shown in Figure 1, this configuration consists of two opposed streams which impinge on each other at a stagnation surface which is approximately centered in the domain via a balance of the flow rates. Additionally, there is a constant pressure that is present in the system, be it the assigned pressure in computational trials, the condition of a pressurized chamber, or the ambient pressure of a rocket combustor. The flow field is characterized by a given local strain rate allowing for a study of the effects of flow straining and residence time. It is well-known that a turbulent flow field is characterized by a wide range of spatial-temporal scales and the associated motion can be visualized as a cascade of eddies. Based on the concept of laminar flamelet, the results of this counterflow configuration can be extended to turbulent system because the turnover time of each eddy can be related to a local strain rate. It is also noted that when replacing the spark plug in an augmented spark system with the proposed catalytic ignition system, the associated configuration will be similar to the one shown in Figure 1, and the resulting ignition kernel from the counterflow will replace the spark as the initial flame source.

Figure 1: Counterflow Configuration with Heated Catalytic Tube for Hot Stream Generation

The counterflow configuration is quasi one dimensional and axis-symmetric. This facilitates experimental testing and would also aid in diagnostics as there is a steady localized planar ignition kernel situated between two opposing streams. Computationally, since it is quasi one dimensional, it can be studied along the stagnation streamline with detailed chemical kinetics, thermodynamic properties, and transport properties included. Because of the level of control and similarity between cases, it allows for a parametric study over variations of the conditions.

The cold stream is the fuel mixture at a lower temperature. The hot stream is the primary source of thermal energy and/or vitiated species into the system as this would be where the catalyst would be located and would yield raised temperatures along with the products of reaction.

The mixtures within the streams can be chosen individually so that by manipulating the concentrations a non-premixed or premixed case can be created. For the purposes of this study, the cold stream will be a mixture of methane and oxygen. The hot stream will be varied from pure nitrogen gas, to nitrogen gas vitiated with different products of catalytic reaction, to mixtures of only catalytically produced products. Since the cold stream is a premixed flow, potentially any gas could be used in the hot stream. So long as it does not introduce too much chemically inhibiting behavior, the ignition could be caused by thermal means. Certain products will introduce some chemically enhancing or inhibiting behavior and the vitiation studies are conducted in order to determine their individual and combined effects.

The hot stream that provides these raised temperatures and products will be a catalytic reactor. There are various types of catalytic reactors but for this study, it will be

limited to small diameter platinum tubes. Since surface catalytic reaction occurs at lower temperatures than gas-phase reaction would normally occur, small diameters allow for the products of surface reaction to permeate the flow and dominate over the gas phase reaction. Using multiple small tubes as one large ignition system would allow for a larger volumetric flow rate with no drop in product or temperature yield. Since methane is relatively nonreactive as compared to other fuels, such as hydrogen, external heating of the catalyst and/or a raised temperature of the incoming gas would be required.

The gas that will be flowed through the catalytic reactor is a mixture of methane and oxygen itself. These will also have to be well mixed upstream. Since the reaction will be assisted by the catalyst, equivalence ratios that are beyond the flammability limits may have the potential to react so a larger range can be tested in order to determine which will have the most beneficial yield for aiding ignition.

1.4: Objectives

Though research into methane and air combustion has been extensively studied and there are some studies that have examined methane and oxygen in a non-premixed situation, the ignition of mixtures of methane and oxygen have not been as thoroughly studied nor have the effects of vitiation on methane and oxygen ignition been examined. While rocket combustion chambers may also exhibit stratification or imperfect mixing, this counterflow configuration allows for a study over all the ranges that may exist.

Studies on the reaction of methane and oxygen on platinum catalysts have occurred but this study seeks to examine specific conditions with limiting factors in mind so as to determine a range of operational capability to employ such a catalyst in a working system. Because of the desire to ease the somewhat difficult methane ignition,

this aspect of the study will attempt to frame a range of concentrations so to determine what is achievable so that these may be further tested.

The counterflow aspect of the study will yield a variety of results across a wide range of conditions. In order to fully establish what is occurring so to best implement these results, not only will the effects of a catalytic hot stream be studied but also the individual effects of the components so that for given conditions an ignition system may be optimized.

1.5: Chapter Breakdown

Chapter 2 will begin by covering the computational methodology, laws, and assumptions that are implemented in order to characterize the behavior of such a catalyst that would typically be used. Chapter 3 will cover similar methods, equations, and assumptions that are utilized for the counterflow configuration to be used. Chapter 4 presents the computational results from a parametric study over various conditions in a catalytic tube. Chapter 5 will cover the results from the counterflow studies. It will start by presenting the baseline results of the ignition of a premixed stream by heated nitrogen, a relatively inert gas in this situation, with systematic variation of equivalence ratio, pressure, and strain. It will then cover the individual vitiation of catalytically produced species. Finally, it will examine the behavior of a heated stream that is comprised entirely of catalytically produced species across a range of pressure conditions to evaluate the applicability of such an ignition system. Lastly, the conclusions that can be derived from the results and the future work that is the natural evolution of this research will be discussed.

Chapter 2: Catalytic Computational Methodology

In order to determine the range of concentrations and temperature of the exit product stream that could be achieved by flowing part of methane/oxygen mixture through a catalytic reactor, a code known as PLUG (Larson, 1996) will be utilized.

2.1: PLUG Code

To simulate the reactions in a catalytic tube, PLUG (Larson, 1996), a code by Sandia National Labs, is used along with CHEMKIN (Kee et al., 1996) and SURFACE CHEMKIN (Coltrin et al., 1996). This code simulates the surface and gaseous reactions that occur in the given system. This model assumes no radial variation in composition, treating it as having perfect mixing in that direction. The axial diffusion is treated as negligible compared to the high speed flow condition. Under certain conditions such as larger diameters and extreme Reynolds numbers, some of the assumptions may start to break down but the purpose of applying PLUG in this implementation is to generate ranges of values for use in the counterflow ignition code.

Below are the governing equations that this code prescribes to.

Continuity Equation:

$$\rho u \frac{dA}{dx} + \rho A \frac{du}{dx} + uA \frac{d\rho}{dx} = a_i \sum_{gas}^{K_g} g_k W_k$$

Species Conservation:

$$\rho u A \frac{dY_k}{dx} + Y_k a_i \sum_{gas}^{K_g} \dot{g}_k W_k = W_k (\dot{g}_k a_i + \dot{\omega}_k A)$$

$$k = 1, \dots, K$$

Energy Equation:

$$\rho u A \left(\sum_{gas}^{K_g} h_k \frac{dY_k}{dx} + \bar{c}_p \frac{dT}{dx} + u \frac{du}{dx} \right) + \left(\sum_{gas}^{K_g} h_k Y_k + \frac{1}{2} u^2 \right) a_i \sum_{gas}^{K_g} \dot{g}_k W_k$$

$$= a_e Q_e - a_i \sum_{bulk}^{K_b} \dot{b}_k W_k h_k$$

Momentum Equation:

$$A \frac{dP}{dx} + \rho u A \frac{du}{dx} + \frac{dF}{dx} + u a_i \sum_{gas}^{K_g} \dot{g}_k W_k = 0$$

Where the $\frac{dF}{dx}$ term is a function of a friction factor related to the Reynolds number

as:

$$\frac{dF}{dx} = a_i * \frac{1}{2} \rho u^2 f$$

Where the Reynolds number determines which f formulation will be used:

$$Re = \frac{Du\rho}{\mu}$$

Laminar ($Re < 2100$):

$$f = \frac{16}{Re}$$

Turbulent, using the approximate Blasius formula:

$$f = .0791Re^{-0.25}$$

Ideal Gas Equation:

$$P\bar{W} = \rho RT$$

Surface site fraction conservation:

$$\dot{s}_k = 0$$

But because the algebraic equations in (previous) are not all independent, for each phase (chosen as species with largest site fraction) one equation must be replaced by:

$$\sum_{phase} Z_k = 1$$

Inlet Conditions:

$x = 0$:

$$T = T_{in}$$

$$P = P_{in}$$

$$u = u_{in}$$

$$Y_k = Y_{k,in}$$

$$Z_k = Z_{k,in}$$

The code simulates a catalytic tube with user prescribed length and diameter. These conditions are represented in Figure 2. In a case with external heating, Q_i , the external heating profile at locations i , is specified. In this study a uniform heat flux Q was assigned over a central length L_Q as shown in the figure. This PLUG code is a steady state model. Further details for PLUG can be found in Larson (1996).

Figure 2: PLUG Representation Diagram

2.2: Chemical Mechanisms

For the surface reactions of the methane and oxygen on platinum, the mechanism by Deutschmann *et al.* (1996) is being utilized. This features 11 surface species and 24 surface reaction steps. The gas-phase mechanism for methane oxidation was taken from GRI-MECH 3.0 (Smith et al., 1999) which contains 53 species and 325 reactions.

Chapter 3: Counterflow Computational Methodology

For the steady-state counterflow ignition study, a quasi-one-dimensional axis-symmetric potential flow formulation (Smooke *et al.*, 1986) code with a two point flame controlling method (Nishioka *et al.*, 1996) is utilized to generate the combustion response curve and capture the ignition turning point.

Figure 3: Flame Response Curve

3.1: Counterflow Code

The counterflow ignition code used is based on the axis-symmetric potential flow formulation of Smooke *et al.* (1986). It studies the behavior primarily in the axial direction along the stagnation streamline. In brief, this code uses a flame controlling continuation method (Nishioka *et al.*, 1996) in order to navigate around the ignition

turning point which is the junction between the lower and unstable branches on the flame response curve as seen in Figure 3. Using a restart profile of a previously solved solution, the code fixes mass fractions of a given key radical at two points on either side of the ignition kernel at a given user-prescribed percentage of the maximum value. While different percentages can be selected, typically both points were controlled at equal percentages in this study. Figure 4 shows a visualization of this. These points are then changed by a given percentage controlled by the user and the new solution is calculated. Changing these points the same positive or negative percentage allow for a move around the curve up or down accordingly while approximately maintaining the same position within the domain. This allows for a steady increase of the controlled radical and mapping of the resulting behavior around the ignition point.

Figure 4: Flame Controlling Method Diagram
 $P = 1 \text{ atm}$, $\phi_F = 1$, $a = 300 \text{ s}^{-1}$, Pure N₂ Counterflow, $T_F = 300 \text{ K}$

The hot stream inlet temperature at the turning point between the lower stable and unstable branches is defined as the ignition temperature. These turning points are the

ignition points and are where profiles in this study will be determined. Examination of the peak mole fractions of the radicals that are not part of the boundary conditions as a function of the temperature yield a working flame response curve as seen in Figure 5. It is seen that while the species concentrations levels are different, the response curves all turn at the same hot stream temperature, indicating the ignition temperature.

Figure 5: Working Flame Response Curve
 $P = 1 \text{ atm}$, $\phi_F = 1$, $a = 300 \text{ s}^{-1}$, Pure N_2 Counterflow, $T_F = 300 \text{ K}$

Typically, the hydrogen radical is the controlled radical but since this study will examine the effects of vitiation of radicals including H, it cannot always be used to control as the maximum may be on the boundary nor have a profile that is otherwise conducive to being controlled at two steady points around the ignition kernel. In the H-radical vitiation cases, the controlling radical has been modified to another that has an easily controllable peak within the computational domain.

The governing equations and boundary conditions utilized are as follows:

Continuity Equation:

$$\frac{dV}{dy} + 2a\rho f' = 0$$

Species Conservation:

$$-\frac{d}{dy}(\rho Y_k V_{ky}) - V \frac{dY_k}{dy} + \dot{\omega}_k W_k = 0$$

$$k = 1, \dots, K$$

Energy Equation:

$$\frac{d}{dy} \left(\lambda \frac{dT}{dy} \right) - c_p V \frac{dT}{dy} - \sum_{k=1}^K \rho Y_k V_{ky} c_{p,k} \frac{dT}{dy} - \sum_{k=1}^K \dot{\omega}_k W_k h_k = 0$$

Momentum Equation:

$$\frac{d}{dy} \left(\mu \frac{df'}{dy} \right) - V \frac{df'}{dy} + a\{\rho_e - \rho(f')^2\} = 0$$

Where:

$$V = \rho v$$

$$f' = \frac{u}{u_e}$$

Boundary Conditions:

$$y = 0$$

$$f' = 1$$

$$Y_k = Y_{k,F} \text{ for } k = 1, \dots, K$$

$$T = T_F$$

$$y = L$$

$$f' = \sqrt{\frac{\rho_I}{\rho_F}}$$

$$Y_k = Y_{k,I} \text{ for } k = 1, \dots, K$$

Internal Conditions:

$$Y(y_{fix1}) = Y_1^*$$

$$Y(y_{fix2}) = Y_2^*$$

Where for this study:

$$Y_1^* = Y_2^* = .7 * Y_{max}$$

The computational domain between two opposing streams is $L = 2$ cm for these trials. The ignition kernels and stagnation point have been centered near 1 cm so that proper behavior can be developed without boundary induced errors affecting the result. The cold stream boundary conditions are assigned at 0 cm and the hot stream at 2 cm. The user assigns the mole fractions of the boundary conditions as well as the temperature of the cold side boundary. A simple diagram of this can be seen in Figure 6. Other conditions that are specified in order to complete the solution is that a constant strain rate in the hot stream is selected as this characterizes the flow field of the domain and a constant pressure is also assigned to the system. Along with the profiles through the domain that are calculated, the response parameters that are determined are the associated mass fluxes and the hot stream temperature when using the two point controlling method.

Figure 6: Counterflow Condition Diagram

Figure 7 shows an example of the resulting temperature and velocity profiles throughout the domain. It can be seen that in the cold stream, the region to the left of the stagnation point which is the point with zero velocity, the temperature rise exists in the region of near zero velocity. There is also an associated change in the nonlinearity of the velocity profile as the composition and density change in this region. The remaining portion of the temperature gradient occurs in the hot stream as the velocity also goes to zero. This loss of thermal energy is what causes the corresponding rise in the cold stream.

Figure 8 shows the species that comprise the flows for this same case. These trends show the diffusion through the stagnation point of all species introduced. Since there is a reacting fuel and oxidizer mixture, there is also some degree of reaction that will consume the species and cause additional falloff. The temperature profile closely matches that of the nitrogen mole fraction as the nitrogen comprises the hot stream and carries the thermal energy into the system.

Figure 7: Example Temperature and Velocity Profiles
 $P = 1 \text{ atm}$, $\phi_F = 1$, $a = 300 \text{ s}^{-1}$, Pure N_2 Counterflow, $T_F = 300 \text{ K}$

Figure 8: Example Temperature and Major Species Profiles
 $P = 1 \text{ atm}$, $\phi_F = 1$, $a = 300 \text{ s}^{-1}$, Pure N_2 Counterflow, $T_F = 300 \text{ K}$

Figure 9 shows the minor species profiles through the domain. While the profile of the H_2 mole fraction covers a large portion of the domain, the ignition kernel is best defined as shown in this case as the region of the mole fraction of CH_3 that is greater than parts per million. This also roughly matches with the area of the domain that begins with

the leveling of velocity and rise in temperature and continues to the extreme of the H radical profile that is also greater than parts per million.

Figure 9: Example Temperature and Minor Species Profiles
 $P = 1 \text{ atm}$, $\phi_F = 1$, $a = 300 \text{ s}^{-1}$, Pure N_2 Counterflow, $T_F = 300 \text{ K}$

3.2: Transport Options

Furthermore, in conjugation with TRANSPORT (Kee *et al.*, 1998), the ignition code has the capability for the user to select a particular transport formulation during the calculations. For molecular diffusion, either mixture-averaged or multi-component formulas can be utilized. Additionally, thermal diffusion, also known as Soret diffusion, effects, can be included. With the mixture averaged formulation, thermal diffusion is only included for the light components in the presence of thermal gradients, i.e. H_2 and H . With the multi-component diffusion formulation, the Soret effects are considered for all species, not solely the light species. These effects can play a large part in altering the

behavior of systems such as these where there are two differently heated streams (Yang *et al.*, 2009). The addition of multi-component or thermal diffusion adds computational time. A set of cases was run on a given machine and the amount of time added by including thermal diffusion was less than 2% of the original run time but the multi-component diffusion trial took *four times* as long. Figure 10 shows and compares the ignition response curve and the turning points for the four possible combinations of these options for a stoichiometric CH_4/O_2 versus hot N_2 case with $P = 100 \text{ atm}$ and a strain rate of $a = 300 \text{ s}^{-1}$.

Figure 10: Comparison of Computed Ignition Response Curves using Different Transport Options.
 $P = 100 \text{ atm}$, $a = 300 \text{ s}^{-1}$, $\phi_F = 1$, Pure N_2 Counterflow

The difference in the mixture averaged turning points is small when comparing having thermal diffusion included or not. The difference in mixture averaged versus multi-component diffusion without thermal diffusion included appears to have a greater

effect, though its actual significance is small. While multi-component diffusion shows the greatest change in required ignition temperature, adding the Soret effects to that formulation reduce this change and bring the required ignition temperature back up to near the same temperatures that the formulations without multi-component diffusion exhibited. While the comparison of turning points shows a difference, examining Figure 10 shows that the disparity of approximately 5 degrees Kelvin from the mixture averaged profile is insignificant compared to the magnitude of the ignition temperature which will be approximately around 1200 K. Even with the expected lowering of ignition temperature, this small difference should be minimal. In addition, all of the spatially resolved scalar profiles at the ignition turning points are indistinguishable. Examining the H radical profile at the ignition kernel similarly shows a very small difference. Because of the minimal effect and the much greater computational time, multi-component diffusion will not be considered for this study.

Figure 11: Analysis of H Radical Diffusion with Soret Effects in Mixture Averaged Diffusion
 $P = 100 \text{ atm}$, $a = 300 \text{ s}^{-1}$, $\phi_F = 1$, Pure N_2 Counterflow

The computed counterflow ignition results presented in the following are based on mixture-averaged approach and include the thermal diffusion effect for the light species of H and H₂. These Soret effects do not add a great deal of computational time and so are included to better the results as the trials with catalytically induced boundary conditions may introduce these light species at a higher concentration that would be present in normal methane/oxygen flame. Figures 11 and 12 both show the effects of this type of diffusion on the overall diffusion flux in the region around the temperature gradient for the same conditions as the ignition turning point. Figure 11 shows the H radical flux. It can be seen that there is some Soret effect that does disturb the pure Fickian induced flux, though the magnitude is one order smaller and only seems to effect about one half of the high flux region where there is a high temperature and notable temperature gradient. This only causes a very minor shift to the hot stream side in H radical peak. Figure 12 shows the similar effects for H₂, though the Fickian diffusion is in the direction towards the cold, premixed stream, is much smaller, so the Soret effect counters this to a greater degree reducing the maximum magnitude of the flux in this direction to about half of its pure Fickian value. The peak of hydrogen occurs near to the peak of the Soret diffusion, so the competing effects eliminate some of the diffusion loss to the cold stream but enhance diffusion up the hot stream essentially slightly shifting the peak to the hot stream. With greater concentrations of these reactive species introduced by a catalyst, including these Soret effects may help portray a more accurate depiction of ignition by catalytic products.

Figure 12: Analysis of H2 Diffusion with Soret Effects in Mixture Averaged Diffusion
 $P = 100 \text{ atm}$, $a = 300 \text{ s}^{-1}$, $\phi_F = 1$, Pure N_2 Counterflow

3.3: Chemical Mechanism

As was used for the gas phase reactions in the PLUG trials, the detailed methane mechanism of GRI-MECH 3.0 (Smith et al., 1999) was utilized for the calculations. This contains 53 species and 325 reactions.

Chapter 4: Catalytic Results

As with most reacting systems, the primary factors that determine the behavior of a catalytically reacting system are pressure, temperature, equivalence ratio, and residence time. In the case of a catalytic tube, residence time is determined by velocity and length of the catalytic surface. Additionally, since a reaction in a catalytic tube would have both surface chemistry and gas phase chemistry, the diameter of the tube would have an effect. Previous works (Boyarko et al., 2005, Volchko et al., 2006, Mento et al., 2006) have given some indication of the behavior of such systems, but this study covers a range of all of these variables in order to determine the possible resultant temperatures and mole fractions that could be achieved as both thermal effects and the chemical kinetics of the various vitiated species have the potential to modify ignition of premixed methane and oxygen.

A common tube length of 10 centimeters was chosen for the study, and an assumption of a tube with no heat loss was employed. While an optimized point might occur earlier and a practical system could use an appropriately shortened catalyst, this length was used in order to capture enough behavior for examination. Likewise, although the resulting product composition and temperature at the tube exit may change to some degree, a catalytic tube could be tuned so that if a greater velocity was required, a longer tube could be used to maintain the same residence time.

For the trials conducted here, a heat flux profile was assigned over the central 7 cm of the total length of 10 cm. The maximum heat flux was 4×10^6 ergs/(cm²·s), with the first and last three millimeters of the heating being linear progressions from no heat flux

to this value. This is chosen as this study treats this as an externally heated catalytic tube. Other options for these conditions are available but with all of the variation in this study, the resultant maximum ranges of mole fractions that will be used in the vitiation studies should encapsulate the ranges produced by other methods.

These are results based on systematic variation. In practice, the melting point of platinum is around 2000 K so some of these results would not be applicable in an actual platinum ignition system. When these results are utilized for the ignition study, this has to be taken into consideration.

4.1: Inlet Velocity Variation

Initially an atmospheric CH_4/O_2 mixture of equivalence ratio $\phi = 5$ was chosen, with an inlet temperature of 600 K and a tube diameter of 0.04 cm. Inlet velocities of 100 cm/s to 500 cm/s were selected. As the mixture reacts within the tube, the velocity will rise. Because of this, these are only initial velocities and residence time cannot simply be calculated as distance divided by inlet velocity. Residence time can be calculated numerically via the relationship:

$$\tau = \int_0^L \frac{1}{u} dx$$

For the range of the inlet velocities studied, they all spike to roughly the same temperature, around 1500 K, when mixture ignition begins, and the spatial distance this sharp rise takes up is similar. This can be seen in Figure 13. After the linear temperature increase range indicative of the heating via the imposed heat flux, there is a non-linear temperature rise prior to a steep rise due to ignition. The beginning of this non-linearity is the point where reactions are beginning to run away in forming products and exhibit a

heat release that has a magnitude that is comparable to the heat flux into the system. The steep rise in temperature is where the system is actively reacting and releasing a great deal of heat. The non-linear rise and the peak behavior all begin and end at roughly the same values for all cases. Changing velocity simply changes how long it takes for these behaviors to occur, not the magnitudes of the peak temperature values reached within the peak. The trend follows as expected, with the slowest case, the one with the greatest residence time, peaking earliest in terms of distance from the inlet.

Figure 13: Temperature Profiles for Velocity Variation through a Catalytic Tube
 $P_{in} = 1 \text{ atm}$, Inlet Temperature = 600 K, $\phi_{in} = 5$

After this spike and the following drop in temperature as endothermic reactions occur, all continue to rise as reactions are still occurring within the system and there is still heat flux into the system. They all tend to plateau at roughly the same distance,

reaching a steady state where the imposed heating ends. Similarly, the mole fractions also level out as the system approaches a steady state behavior. While they do level, it is seen that H and CH₃ concentrations still fluctuate, so even though there is no heating in this section some reactions are occurring. This is shown via the H radical mole fractions in Figure 14. While this leveling trend is common, the faster speeds level out to lower temperatures and smaller concentrations of H radical, the continuing reactions are not allowed to carry on as long. In order to implement these results, a decreased velocity would result in higher temperatures and radical concentrations, but can potentially exceed the melting point of the catalyst.

Figure 14: H Radical Profiles for Velocity Variation through a Catalytic Tube
 $P_{in} = 1 \text{ atm}$, Inlet Temperature = 600 K, $\phi_{in} = 5$

4.2: Inlet Temperature Variation

The resultant temperature profiles along the tube by varying inlet temperatures are compared in Figure 15. The range that selected varies from room temperature to 900 K. For relatively lower inlet temperatures, the atmospheric results show that the initial linear rise in the temperature profile leads to a larger rise that starts at around 800 K and begins a near vertical jump at 900 K. The 900 K inlet temperature case eliminates this linear temperature increase; the initial temperature is high enough that only a minimal amount of residence time is required before this thermal runaway, it does not need the heat flux the lower temperature cases require.

Figure 15: Temperature Profiles for Initial Temperature Variation through a Catalytic Tube
 $P_{in} = 1 \text{ atm}$, Inlet Velocity = 300 cm/s, $\phi_{in} = 5$

While the eventual temperatures reached differ downstream, the magnitude of the initial temperature peak for all appears unaffected by the inlet temperature. Like the inlet velocity variation trials, the methane oxidation behavior begins at roughly the same temperature, it just requires a longer time, i.e. it occurs more downstream from the inlet, for this condition to be achieved with lower inlet temperatures. As in the inlet velocity variation, there is also varying radical concentrations as seen in Figure 16 and Figure 17, producing less H at the tube exit with lower inlet temperatures. Note that the few scattered points of CH_3 that appear near 4 and 2 centimeters respectively, the primary reaction zone where the temperature spikes also occurred, are just evidence of this spike in reaction. The concentration starts below the lower axis then spikes as shown followed by a dip below the shown threshold on the graph before rising again with the continued heat flux and reaction. While this is a spike, it is a very thin zone that would be difficult to control to near the outlet, it is why the trials shown have a longer length, so as to capture the more steady downstream conditions. The remaining CH_4 and the produced H_2 have comparable concentrations in both 500 K and 700 K runs, though O_2 is consumed to a greater extent at 700 K. The higher inlet temperature condition lends itself to the production of more H and CH_3 radicals. The overarching trend is that higher inlet temperatures will consume more O_2 in exchange with the production of more radicals.

Figure 16: Mole Fraction Profiles Through a Catalytic Tube with Initial Temperature = 500 K
 $P_{in} = 1 \text{ atm}$, Inlet Velocity = 300 cm/s, $\phi_{in} = 5$

For a practical usage, a longer catalytic tube would require the mixture to be less hot initially to achieve exit temperatures over 1300 K should energy conservation be an issue. This may have less beneficial radical production, though the requisite amount of radicals to use a catalytic igniter will be reviewed later. Although shorter catalysts can be used in conjunction with greater heating or preheating of the gas, the upper limit of the melting point must be minded.

Figure 17: Mole Fraction Profiles Through a Catalytic Tube with Initial Temperature = 700 K
 $P_{in} = 1$ atm, Inlet Velocity = 300 cm/s, $\phi_{in} = 5$

4.3: Pressure Variation

While the effect of pressure on ignition will be further examined in the counterflowing condition case, changing pressure in the catalytic reactor has a pronounced effect on its behavior. While at an inlet temperature of 500 K, the 1 atm case would react at a location within the tube and reach a high exit temperature, this was not the case under elevated pressures with the other conditions held the same. More energy was required in order to induce reactions within the tube; either a higher temperature or a greater residence time within the tube section with the heat flux. As seen in Figure 18, a combination of greater residence time and higher initial temperature was needed in order to obtain proper reaction within the tube. A higher temperature could be used on its own,

but with the same heat flux into the tube, it is more sensitive to change and would require a very high temperature. As shown, if the temperature is that high, it will react quickly within the tube, near to the inlet. In order to keep the temperature down, slower speeds or a much longer tube would be required. Additionally, a greater heat flux could be added but this would be similar to raising the temperature and such energy addition is not always able to be achieved. For the following trial, the inlet velocity was greatly reduced, down to 15 cm/s.

Figure 18: Temperature Results as a Function of Pressure Variation in a Catalytic Tube
 $\phi_{in} = 5$

Component	$P_{in}=50$ atm	$P_{in}=100$ atm
H ₂	4.40E-01	3.95E-01
H	1.31E-05	8.27E-06
H ₂ O	1.08E-01	1.26E-01
CH ₃	1.10E-04	9.34E-05
CH ₄	1.82E-01	2.20E-01
CO	2.34E-01	2.25E-01
CO ₂	1.70E-02	2.14E-02
CH ₂ O	2.97E-06	4.83E-06
CH ₃ OH	1.18E-06	1.87E-06
C ₂ H ₂	8.56E-03	3.90E-03
C ₂ H ₃	1.71E-06	1.03E-06
C ₂ H ₄	9.64E-03	8.28E-03
C ₂ H ₅	2.78E-06	3.15E-06
C ₂ H ₆	5.01E-04	8.01E-04
CH ₂ CO	8.76E-06	9.56E-06
C ₃ H ₇	3.42E-06	7.26E-06

Table 1: Resultant Species Mole Fractions from a Catalytic Tube at Pressures of 50 and 100 atm $\phi_{in} = 5$, $V_{in} = 15$ cm/s, $T_{in} = 650$ K.

Table 1 gives approximate mole fraction values of what the primary (greater than ppm level) species would be at the tube exit for two inlet pressures, 50 and 100 atm. Here, the inlet temperature is kept constant at 650 K. Even though there is a 50 atmosphere difference in pressure, the results in mole fractions remain similar to each other as did the temperatures, with only about a 2 degree Kelvin difference at the exit. The peak temperature after the sharp rise is less than 30 degrees apart, though the 100

atm case does not show a peak and quick drop that the other results showed. Rather, it showed a slower decrease from this high point and that decrease continued to the exit. The 50 atm case reacted much sooner in the domain than the 100 atm case did, with another 3 cm of delay in the 100 atm case. Higher pressures mean greater density; essentially a greater mass flow which would require more energy to bring that flow to the same ignition temperature. In terms of yield, though the results were similar, the higher pressure favors the larger hydrocarbons slightly. Major species had similar orders of mole fractions but the larger minor species have greater concentrations at the higher pressures. Other condition variation, as demonstrated already, can vary the concentration levels and yield.

Implementing this into a catalytic ignition system would require a higher inlet temperature capability or greater heat flux as speeds cannot always be reduced to those tested in this study. Using an igniter in this regime would result in less variation over the key species yield as seen with the large pressure change and small change in resultant mole fractions. The degree of change in temperature and composition by altering other factors is somewhat nullified at higher pressures so larger changes would be required should different vitiated products be needed to enhance ignition. These results indicate that at higher pressures a potential catalytic system would not be as energy saving as at low pressures.

Figure 19: Temperature Profiles through a Catalytic Tube as a Function of Equivalence Ratio
 $P_{in} = 1 \text{ atm}$, $V_{in} = 300 \text{ cm/s}$, $T_{in} = 600 \text{ K}$

4.4: Equivalence Ratio Variation

Using $P_{in}=1 \text{ atm}$, inlet velocity of 300 cm/s , and inlet temperature of 600 K , the temperature profiles of various equivalence ratios are calculated and compared as shown in Figure 19. In terms of the overall reactivity, regardless of the equivalence ratio, all mixtures showed similar trends in the initial linear rise of temperature caused by the heat flux. While the near stoichiometric conditions took longer to reach their peak temperature than fuel rich mixtures, they had more instantaneous behavior at the spike in reaction and reached higher temperatures. The fuel rich mixtures exhibited an earlier rise but it was not as steep and leveled off to lower temperatures. The leanest mixtures ($\phi < 0.1$) took

the longest to reach runaway as there was less fuel to react with, it naturally took longer for the appropriate concentration of radicals to build up.

Lean mixtures would not be suggested for use in an ignition system. While the temperature did exhibit a rise, it took an excessively lean mixture to keep that from passing the melting point. As shown with the other variation trials, changing other conditions may have a small effect on the resulting temperature, but the peak values tend to not be affected; equivalence ratios that result in high temperatures need to be avoided. While O_2 may aid ignition in counterflow, equal concentrations of H_2 are more beneficial as will be demonstrated in the vitiation section. Mixtures this lean would be lacking in concentration of many of the beneficial hydrocarbons. Additionally, balancing the degree of richness of the mixture would be required.

Figure 20: Mole Fraction Profiles of Key Components through a Catalytic Tube with Inlet $\phi = 5$
 $P_{in} = 1 \text{ atm}$, $V_{in} = 300 \text{ cm/s}$, $T_{in} = 600 \text{ K}$

Even though both cases are in the rich regime, Figure 20 and Figure 21 show that being more towards stoichiometric yielded more H_2 , radicals, and less inhibitive H_2O . While it became closer to stoichiometric, the temperature rose as it nears or surpasses the melting point. These two cases were chosen to compare as they are both under the melting point and physically possible cases. Equivalence ratio of $\phi = 5$ would be the ideal of these runs as it has a distinct temperature rise that is high but safely away from the melting point of platinum and generates beneficial product mixtures.

Figure 21: Mole Fraction Profiles of Key Components through a Catalytic Tube with Inlet $\phi = 10$
 $P_{\text{in}} = 1 \text{ atm}$, $V_{\text{in}} = 300 \text{ cm/s}$, $T_{\text{in}} = 600 \text{ K}$

4.5: Tube Diameter Variation

Lastly, the diameter of the tube can have an effect. The proportion of surface to gas phase chemistry will change affecting the overall yield. A larger tube volume takes longer to heat for given inlet temperature and imposed heat flux. The temperature profiles

of the variation of tube diameters, ranging from 0.04 to 0.12 cm, shown in Figure 22, exhibit this behavior as well as the appropriate catalytic behavior. Though the extent of surface chemistry and gas-phase chemistry remains the same, as indicated by similar trends, ignition temperatures, and peak temperatures, it just takes longer with a larger tube. With similar mixtures to react on the surface and the near perfect radial diffusion assumption causing the chemistry within the gas-phase to be uniform, the only major differences in the systems are two specific ratios. These two ratios both correspond to surface effects versus volumetric effects. First, there is more mass flow for the heat flux to be absorbed into in order to bring it to the required temperature. As the diameter is increased, the surface area rises in a linear manner, $\pi * L * D$, yet the volume rises according to $\pi * L * \frac{D^2}{4}$. The heat flux through the surface does increase but the volume to be heated increases by an additional order of magnitude. Secondly, there are the effects of chemistry. The amount of surface chemistry increases as did the flux as there was a greater surface area, yet there was once again a greater increase in amount of gas within the tube to be reacted that would keep concentrations lower. The same chemical steps will occur, it will just take longer as the chemistry is a function of concentration, which will take longer to rise to the corresponding levels.

Because of these similarities, the resultant temperature spikes all occur starting at the same temperature and ending at the same temperature. The H radical profiles also show this same behavior. While there is a small increase with increasing diameter, the continuing heating will have some effect as the rises occur in areas with different imposed heat flux, but the overall magnitudes and trends of the runaway spike are

similar. Practically speaking, a larger diameter will require more residence time or heating to react.

Figure 22: Temperature Profiles through a Catalytic Tube as a Function of Tube Diameter
 $P_{in} = 1 \text{ atm}$, $V_{in} = 300 \text{ cm/s}$, $T_{in} = 500 \text{ K}$, $\phi_{in} = 5$

4.6: Condition Selection and Vitiation Concentrations

As has been discussed, a wide range of gaseous species concentrations can be achieved. The orders of the maximums of the tested criteria have been accumulated and are listed in Table 2. While manipulating multiple conditions and going to further extremes than tested may yield even greater concentrations of any given radical or product, these are the typical ranges that have been observed and should encapsulate most of the possible values.

Component	Mole Fraction	Component	Mole Fraction	Component	Mole Fraction	Component	Mole Fraction
H2	0.75	H	0.05	O	0.05	O2	1.0
OH	0.01	H2O	0.25	HO2	0.001	H2O2	0.001
CH	2.5E-5	CH2	5.0E-4	CH3	0.1	CH4	0.75
CO	0.5	CO2	0.5	HCO	5.0E-4	CH2O	0.01
CH2OH	1.0E-4	CH3O	5.0E-5	CH3OH	5.0E-4	C2H	1.0E-4
C2H2	0.05	C2H3	5.0E-4	C2H4	0.01	C2H5	5.0E-4
C2H6	5.0E-4	HCCO	5.0E-4	CH2CO	5.0E-4	HCCOH	5.0E-4
C3H7	1.0E-5	C3H8	5.0E-6	CH2CHO	5.0E-5	CH3CHO	5.0E-4

Table 2: Maximum Mole Fraction Data for Vitiating Testing

While testing these individually will reveal their effects on ignition in the counterflow configuration, most of these would not exist solely. Equipment like catalytic igniters or using pre-combustion would yield a variety of products that would continue to react with each other and have a group effect on the ignition kernel. In order to test this grouping effect, a specific trial had to be chosen. This will be used as the boundary condition for a counterflow ignition trial to test this behavior.

4.7: Catalytic Igniter Output

The chosen full profile was selected as an atmospheric pressure case. The inlet temperature is 500 K, inlet velocity is 300 cm/s, $\phi = 5$, and tube diameter is 0.04 cm. Figure 23 and Figure 24 show the temperature distribution and resultant mole fraction profiles of key radicals. At 9.3 cm, it has a temperature of 1520 K, below the melting point of platinum, having not exceeded the melting point at any location in the reactor, as

well as a mole fraction profile that has eight species with greater than ppm level concentrations. At this location, H_2 and CO are at a high, with H_2O and CH_4 having decreased off of their maximums. Though CO_2 is present and O_2 has reached a minimum, CH_3 and H radicals are present and above ppm level. As the effects of sub-ppm level concentrations are negligible in individual vitiation testing, anything below one part per million has been excluded. The mole fractions used for assessing the combined and individual effects in the counterflow ignition runs are listed in Table 3. Full trials were run to determine the turning points for incremental mole fractions from ppm level on up to the previously mentioned maximum values so these will also be tested individually with the balance being N_2 .

Figure 23: Temperature Profile of Chosen Catalytic Case:
 $P_{in} = 1 \text{ atm}$, $\phi = 5$, $V_{in} = 300 \text{ cm/s}$, $T_{in} = 500 \text{ K}$

Figure 24: Profiles of Key Species Mole Fractions of Chosen Catalytic Case:
 $P_{in} = 1 \text{ atm}$, $\phi_{in} = 5$, $V_{in} = 300 \text{ cm/s}$, $T_{in} = 500 \text{ K}$

Component	Combined Mole Fraction	Individual Mole Fraction	Component	Combined Mole Fraction	Individual Mole Fraction
H2	5.675E-01	5.0E-01	H	1.859E-06	1.0E-6
O2	1.240E-03	1.0E-03	H2O	2.282E-02	1.0E-2
CH3	7.636E-06	1.0E-5	CH4	1.133E-01	1.0E-1
CO	2.888E-01	1.0E-01	CO2	6.363E-03	1.0E-2

Table 3: Specific Mole Fraction Data for Combined Testing and Approximate Mole Fraction Data for Individual Testing

Chapter 5: Counterflow Results

As in the PLUG results, ignition in the counterflowing configuration is dependent on the same parameters that most combustion systems are functions of. The pressure of the system and the strain rate, which prescribes the characteristic flow time of the system, are two such controlling conditions whose effects will be examined. The boundary temperature of the cold premixture stream can also have an effect but will not be studied in these trials. The premixture temperatures for all cases in this study are 300 K. The temperature of the hot stream will be determined in order to determine the critical ignition condition. The equivalence ratio of the cold stream will be varied from stoichiometric through fuel rich conditions as these conditions would be typically employed in a methane rocket engine. The hot stream will be initially pure N_2 in order to establish a baseline so that the effects of vitiation and a combined catalytically-reacted profile can be examined and compared. The model will be as discussed and as shown in Figure 6, with the distance being referenced as distance from the cold stream.

5.1: Cold Stream Equivalence Ratio Variation

For the purpose of using a catalytic igniter for typical propulsion applications, the mixtures that would be ignited are most commonly rich mixtures. In order to determine the effects of the cold stream equivalence ratio variation, trials were run with the same conditions at 100 atm and $a = 300 \text{ s}^{-1}$ with cold stream equivalence ratio in the range of $\phi = 1.0 - 3.0$ and the hot stream being pure N_2 . It is found that the hot stream boundary, indicating the minimum ignition temperature increases with increasing equivalence ratio, varying from 1240 K to 1370 K with around 60 degree Kelvin increases for every ϕ

increase as seen in Figure 25. Figure 26 compares the temperature profiles at the ignition turning point for three different equivalence ratios in the ignition kernel region. Other than some staggering due to the numerical addition of further grid point, the trends are similar, only leveling earlier with the lower requisite temperature for the stoichiometric case but the gradient occurs in all cases in approximately the same spatial location.

Figure 25: Comparison of Temperature Profiles at the Ignition Turning Point for Three Cold Stream Equivalence Ratios
 $P=100$ atm, $a = 300$ s⁻¹, and hot stream: 100% N₂

Figure 26: Ignition Kernel Comparison of Temperature Profiles at the Ignition Turning Point for Three Cold Stream Equivalence Ratios
 $P=100$ atm, $a = 300$ s⁻¹, and hot stream: 100% N₂

Figure 27 compares the H radical profiles in the reaction zone at the corresponding ignition turning point for three equivalence ratios. While the peak H mole fraction is also seen to increase with increasing ϕ , the peaks are in roughly the same position and follow the same trends. With the increase from stoichiometric to $\phi = 3$, the radical concentration is almost one order of magnitude greater. The H radical profiles as the cases become fuel rich also tend to broaden away from the peak. Since these higher temperatures are required for the more rich cases and there is a greater proportion of hydrogen yielding species, greater radical peaks will develop. The created and diffusive region of H Radical around the peak will increase accordingly.

Figure 27: Comparison of H Radical Mole Fraction Profiles at the Ignition Turning Point for Three Cold Stream Equivalence Ratios $P=100$ atm, $a = 300 \text{ s}^{-1}$, and hot stream: 100% N_2

Since the initial difference in these trials is the equivalence ratio, it follows that the trends in local equivalence ratio will give rise to the important behavior in the system. Figure 28 shows the local equivalence ratio evolution from the non-reacted incoming flow through the ignition kernel. The behavior of the rich cases initially shows a dip towards stoichiometric as the fuel breaks at a greater rate than the oxygen as shown in Figure 29. Originally, both consumption rates are negligible even though the oxygen consumption is greater. When the streams approach the ignition kernel, the methane consumption becomes greater for both stoichiometric and rich cases. As it approaches the

peak, these values become greater and similar. There is a small region where oxygen is consumed at a greater rate. At peak and post-peak the methane consumption overcomes again as more is present for both cases as more oxygen has been consumed. The rich case has much greater methane consumption further along the domain as there was unreacted fuel that diffused through the ignition kernel. The less initial oxygen in the progressively richer cases approaches zero concentration quicker causing the greater slopes.

Figure 28: Comparison of Local Methane/Oxygen Equivalence Ratio at the Ignition Turning Point for Three Cold Stream Equivalence Ratios
 $P=100$ atm, $a = 300$ s⁻¹, and hot stream: 100% N₂

Figure 29: Molar Consumption Rates for Two Cold Stream Equivalence Ratios at the Ignition Turning Point, $P=100$ atm, $a = 300 \text{ s}^{-1}$, and hot stream: 100% N_2

5.2: Pressure Variation

Pressure effects will change a variety of things in combustion, from density, to diffusion capability, to molecular collision speed and resulting reaction rates. All these individual effects will have a great deal of influence on the overall requisite ignition temperature and ignition kernel profile.

Figure 30 compares mole fraction profiles of several species at the ignition turning point under pressures of 1 and 100 atm, corresponding to ignition temperatures of 1695 K and 1240 K, respectively. For the same strain rate of $a=300 \text{ s}^{-1}$, it is seen that the overall reaction zone becomes narrower as pressure is increased. There are lower concentrations of the generated H radical and molecular hydrogen at higher pressure due to the lower temperature.

Figure 30: Comparison of Species Mole Fraction Profiles at the Ignition Turning Point
 $P=1$ and 100 atm, for pure N_2 vs. $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

The thinning is expected as the mixing layer thickness in a counterflow configuration scales inversely with $\sqrt{pa}$ (Sun et al. 1996). The ignition kernel width at higher pressure in Figure 30 is evidence of this, the strain was kept constant in both cases but the high pressure case has a much higher density. While Figure 11 and Figure 12 showed the H radical and molecular hydrogen diffusion profiles at 100 atmospheres, Figure 31 and Figure 32 demonstrate the same at 1 atm. Since the flux is a function of both the amount of a given component and how fast it goes, the greater by order of

magnitudes fluxes at 1 atm are a result of having the greater generated concentration of species and a larger mass diffusivity. Even though the higher pressure would have a greater density that would increase the mass based flux of a species, the other effects counter this significantly.

Figure 31: H Radical Diffusion Flux Profile
 $P=1$ atm, for pure N_2 vs. $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

Figure 32: H₂ Diffusion Flux Profile
 $P=1$ atm, for pure N_2 vs. $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

The chemistry that will be affected by the pressure change will be examined with the catalytic chemistry introduced as that may also change at high pressure, but, other than the chemistry, ignition is also dependant on this convection and diffusion. Figure 33 shows the overall effect that these aspects of raising pressure induce on the ignition temperature. The requisite ignition temperature for $P = 1$ atm case is ~ 1695 K, which is much higher than ~ 1240 K of the $P = 100$ atm case. The overall thinning of the reaction zone is also reflected in the temperature profile as well.

Figure 33: Temperature Profiles at the Ignition Turning Point for pure N_2 vs. $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

In terms of ignition capability, the lower requisite temperatures at higher pressures are beneficial. As discussed earlier, under various pressures, high temperatures

can be reached with a catalytic igniter. Even though the catalyst may require a higher inlet temperature than at lower pressures, the inlet temperatures of the catalyst under these conditions are still lower than the requisite heated N_2 temperatures in the counterflow baseline case. The catalysts also produced exit temperatures higher than the N_2 hot stream temperature across this range. So long as the effects of the catalytic product gases do not inhibit ignition and make it require an even higher ignition temperature, the concept of catalytic igniter would be feasible. This result will aid a catalytic ignition system as the onset of ignition is usually associated with a pressure rise; the igniter will still be able to function should there be a higher pressure present in the system and potentially more efficiently.

Figure 34: H Radical Profile at the Ignition Turning Point as a Function of Strain, $P = 1 \text{ atm}$, for pure N_2 vs. $\Phi_F = 1.0$

5.3: Strain Rate Variation

In this system, strain rate determines the flow field and these aerodynamic effects can have an impact on ignition. Higher strain rates have higher velocities at the inlets for a given separation distance between two opposing jets, and hence results in shorter residence times within the ignition kernel. In order to study these effects, trials were run with the pressure as 1 atmosphere. Figure 34 compares the mole fraction profiles of H radical at the ignition turning point under different straining conditions. It is noted that the ignition temperature increases with increasing straining. The higher strain rate cases have a higher peak concentration and the lower strain rate cases show some broadening. This causes the side of the peak towards the hot stream to eventually have a greater concentration under lower strain conditions even though the cold side profiles terminate at a similar location. This broadening also does not appear significant enough to have considerably reduced the peak values, the smaller peaks are a result of the lower temperature. Figure 35 shows that the primary cause of this disparity in the peak values is the difference in the production rates of the H radical. It is further noted that the requisite ignition temperatures have a variation of less than 100 degrees K with the higher strain rates requiring the greater ignition temperatures; ~ 1630 K at $a = 150 \text{ s}^{-1}$ and ~ 1695 K at $a = 300 \text{ s}^{-1}$. These cases do not exceed the possible temperatures that a system like a catalytic igniter could provide.

The lower incoming velocities, shown in Figure 36, associated with a lower strain allow for ease of diffusion of thermal energy which is why there is a greater temperature further up the premixed stream though the hot stream is cooler. Diffusion of thermal energy is proportional to $\sqrt{(\alpha/a)}$ and while the concentrations will be somewhat different

in the ignition kernel, changing α to a small degree, examining the production rates yields an idea of where this ignition kernel would be, from 0.9 to 1.2 cm. The temperature gradient passes through this kernel into the cold stream where the composition would be the same and there is still a pronounced difference confirming that the difference in straining is the primary cause for the difference in thermal profiles, not any difference in chemistry. The stagnation points match up with similar values in temperature and onset of reaction between the cases though the stagnation point is in different locations due to the differences in incoming velocity and associated residence time.

Figure 35: Temperature and H Radical Production Rate as a Function of Strain
P = 1 atm, for pure N₂ vs. $\phi_F = 1.0$

Figure 36: Comparison of Velocity Profiles at the Ignition Turning Point for Varying Strain Rates
 $P = 1 \text{ atm}$, for pure N_2 vs. $\phi_F = 1.0$

For a catalytic ignition system, these results show a scaling of ignition temperature with respect to straining for the conditions investigated. The requisite ignition temperature did not have a wide variation and what variation it exhibited should be within the temperature variation capabilities of a catalytic igniter regardless of the cause of straining.

5.4: Hot Stream Vitiation

For the baseline case of heated nitrogen versus the premixed methane/oxygen at atmospheric pressure with $\phi = 1$, and $a = 300 \text{ s}^{-1}$, the ignition temperature was shown to be around 1695 K. The set and range of species for vitiation was established by the PLUG trials. The modified ignition temperatures due to each vitiated species maximums are listed in Table 4, with those having a value less than the baseline value aiding ignition and those with a value higher then inhibiting.

Component	Mole Fraction	T _{ig} (K)	Component	Mole Fraction	T _{ig} (K)	Component	Mole Fraction	T _{ig} (K)
H ₂	0.75	1077.72	H	0.05	1001.79	O	0.05	862.80
O ₂	1.0	1235.25	OH	0.01	1474.13	H ₂ O	0.25	1708.56
HO ₂	0.001	1659.05	H ₂ O ₂	0.001	1665.01	CH	2.5E-5	1692.21
CH ₂	5.0E-4	1678.77	CH ₃	0.1	805.77	CH ₄	0.75	1742.67
CO	0.5	1650.51	CO ₂	0.5	1707.64	HCO	5.0E-4	1685.20
CH ₂ O	0.01	1570.74	CH ₂ OH	1.0E-4	1690.91	CH ₃ O	5.0E-5	1692.96
CH ₃ OH	5.0E-4	1679.16	C ₂ H	1.0E-4	1685.16	C ₂ H ₂	0.05	1569.87
C ₂ H ₃	5.0E-4	1676.83	C ₂ H ₄	0.01	1526.09	C ₂ H ₅	5.0E-4	1677.63
C ₂ H ₆	5.0E-4	1676.19	HCCO	5.0E-4	1684.99	CH ₂ CO	5.0E-4	1683.71
HCCOH	5.0E-4	1697.29	C ₃ H ₇	1.0E-5	1694.32	C ₃ H ₈	5.0E-6	1694.29
CH ₂ CHO	5.0E-5	1692.13	CH ₃ CHO	5.0E-4	1690.29			

Table 4: The Resulting Ignition Temperatures due to Individual Vitiated Species in the Hot Stream for P = 1 atm, Hot N₂ with Vitiating vs. $\phi = 1.0$, and $a = 300 \text{ s}^{-1}$

Only a few species of those included in the mechanism were inhibitors. H₂O and CO₂, products of methane combustion, are expected to be so. These are relatively inert species, have high third-body collision efficiencies, and because of dilution their vitiation requires higher ignition temperatures. However, even at large concentrations the effect is less than a 15 degree Kelvin increase, which should be evenly compensated for by one of the many other ignition promoting species in a full catalytically introduced profile of species. CH₄ also inhibits and to the greatest extent of these. Introducing more CH₄ to the ignition kernel would make it more fuel rich and require a higher temperature, similar to raising the cold stream equivalence ratio.

A few species had a very limited effect, less than a one degree Kelvin change. All species on the parts per hundred thousand and parts per million scales had a less than 4 degree Kelvin change. Species with concentrations on the 10⁻⁴ scale exhibited changes

approaching 20 degrees Kelvin. While individually this may not be that large of an effect, if some were included and each effect was additive, it could potentially lower the ignition temperature of a mixture significantly.

The other components that had larger concentrations had more pronounced effects. While the greater concentrations tended to correspond with larger drops, the largest drops come from H and O radicals which had only a mole fraction of 0.05. This behavior is logical as it is essentially delivering a radical pool directly to the ignition kernel. While upstream recombination may occur to some extent, the products, such as H_2 and O_2 , can also be beneficial to ignition. Most of these other components are radicals which have similar effects of delivering a radical pool to the ignition kernel to enhance ignition. Of the initial reactants, CH_4 inhibited ignition but O_2 enhanced it significantly.

Figure 37: Comparison of Ignition and Maximum Temperatures at the Ignition Turning Point of H Radical and H₂ Vitiatio Trials for $P = 1$ atm, pure N₂ vs. $\phi = 1.0$, and $a = 300 \text{ s}^{-1}$

Figure 37 shows the progressive lowering of ignition temperature with increasing vitiatio of two species, molecular hydrogen and H radical. H radical shows a noticeable drop in ignition temperature at a smaller concentration and also shows a large divergence between the ignition temperature determined by the hot stream boundary temperature and maximum temperature reached in a domain. This behavior is shown in detail in Figure 38. Unlike the previous trials against pure nitrogen, there is a difference between the

maximum temperature and hot stream temperature. It is seen that there is a great deal of change in the mole fraction of H radical, with a corresponding growth of molecular hydrogen. H radical is naturally unstable and since the only other component with which it could combine with, other than itself, would be nitrogen, a relatively nonreactive species. It follows that using the other H radical, molecular hydrogen, and nitrogen as the third body, it primarily recombines to form hydrogen via the reaction:

Figure 38: Profiles of Temperature, H₂, and H Radical at the Ignition Turning Point for the Case with H Radical Vitiatio of Mole Fraction = .01 in N₂ vs. $\phi = 1.0$ for $P = 1$ atm, and $a = 300 \text{ s}^{-1}$

The rates of the other reactions that occur in this region are not more than approximately 1% of the rate of the recombination reaction.

Figure 39 shows the heat release differences in the pure case versus the vitiated case. While there is some negative, exothermic, behavior in the normal case, this is along the temperature rise, not creating a peak. The vitiated case has exothermic behavior in the same region as in the pure case, though it is to a much greater degree and wider, resulting in a peaking of temperature; the heat release overcomes the temperature gradient. Additionally, the recombination of H into hydrogen molecules is also an exothermic process, causing the temperature rise along the hot stream prior to the ignition kernel.

**Figure 39: Heat Release Rate Profiles of Counterflow Ignition at Ignition Turning Point Comparing a Pure N₂ Counterflow Case with a .01 Mole Fraction H Radical Vitiated Case for $\phi_F = 1.0$, for P = 1 atm, and $a = 300 \text{ s}^{-1}$
Note: Positive is Endothermic**

The molecular hydrogen vitiation also had a greatly reducing effect on ignition temperature. It did not show the degree of exothermic behavior that would cause a difference between ignition and maximum temperature that was witnessed with the H radical. This is because hydrogen is a relatively stable species as opposed to being a

radical; it would still have to undergo the largely endothermic initiation reactions first whereas the H radical is already broken down. Where initiation reactions are generally endothermic, this H radical will react along the pathways that have an overall heat release. The methane and oxygen species will still need to be initiated and their consumption process will still have some endothermic processes that will require the thermal energy but with the excess H radical being conducted to and diffusing into the ignition kernel it will help to stimulate some of these reactions. Molecular hydrogen itself is a fuel though, and one that ignites at a lower temperature than methane. Because of this, it will primarily remain unreacted up to the ignition kernel, unlike the H radical, and then diffuse into it creating a mixture that would have a lower ignition temperature though not overall being largely exothermic.

The dominant reactions that account for the heat release in both cases are somewhat different because of the different chemistry induced by the vitiation. Table 5 shows the three dominant reactions for both the non-vitiated case and the same H Radical vitiated case at their respective peaks in heat release, which are at central locations in the ignition kernels. The reactions indicated by the gold are those that had the greatest release, green are the two following, and the red are for comparison as they are less important for that case. For the non-vitiated case, the peak reaction has a heat release of almost an order of magnitude less as similarly previously shown in the cumulative graph. Even the lesser important reactions in the vitiated case still have magnitudes that rival the heat release of the major contributing reactions in the non-vitiated as seen in reaction 98. This reaction has a greater heat release with vitiation even though it is not one of the top three contributing for that case yet is for pure case. Also for the non-vitiated case, the

methyl radical chemistry is dominant but a major source of heat release is the formation of water. The methyl radical chemistry is even more enhanced in the vitiated case with the top three reactions being the consumption of it. The greatest heat producing reaction is the interaction of the methyl radical with the vitiated species, H radical. While all the other reactions were similar magnitude or one order different, this reaction was enhanced a thousand times. While the largest reaction in the pure case accounted for half the heat release and the top three reactions accounted for almost all, the major reaction in the vitiated case only accounted for a fourth and the sum only about a half of it. Because of this, more heat releasing reactions had to have been enhanced or endothermicity reduced. While the temperatures at these specific peaked points, 1524.139 Kelvin for the vitiated case and 1475.345 K for the pure, are different and higher temperatures can change chemistry, the much greater H radical concentration that diffuses into the ignition kernel is what exaggerates this difference over all the others.

		Pure N ₂ Heat Release Rate	H Radical Vitiated Heat Release Rate
Reaction #	Corresponding Reaction	ergs/ sec*cm ³	ergs/ sec*cm ³
10	O+CH ₃ <=>H+CH ₂ O	-1.64E+06	-6.99E+07
52	H+CH ₃ (+M)<=>CH ₄ (+M)	-2.43E+05	-1.18E+08
98	OH+CH ₄ <=>CH ₃ +H ₂ O	-1.11E+07	-2.38E+07
156	CH ₃ +O ₂ <=>OH+CH ₂ O	-6.65E+06	-1.64E+06
158	2CH ₃ (+M)<=>C ₂ H ₆ (+M)	-2.44E+07	-8.41E+07

Table 5: Dominant Reactions for Heat Release at Heat Release Peak at Ignition Turning Point Comparing a Pure N₂ Counterflow Case with a .01 Mole Fraction H Radical Vitiated Case for $\phi = 1.0$, for P = 1 atm, and a = 300 s⁻¹

Note: Gold is Maximum, Green are the Next Two Greatest, and Red is for Comparison with Other Case
Note: Positive is Endothermic

Figure 12 showed the diffusion patterns of hydrogen in a non vitiated stream, though at 100 atm. It was commented on how it primarily diffuses to the hot stream direction. Figure 40 shows the H₂ profile and resulting flux for a H₂ vitiated case. The peak value of hydrogen in a non-vitiated case is much lower than the concentration introduced to the domain in the vitiated case so it is overcome and the diffusion is purely to the cold side and of a much higher order of magnitude, creating this mixed fuel case that lowers ignition temperature.

Figure 40: Profiles of H₂ Mole Fraction and Diffusion Flux for the .5 Mole Fraction H₂ Vitiated Case with $\phi_F = 1.0$ for $P = 1$ atm, and $a = 300$ s⁻¹

Figure 41: Mole Fraction Profiles for .5 Mole Fraction H_2 Vitiating Case and Pure N_2 for $\phi_F = 1.0$, $P = 1$ atm, and $a = 300 \text{ s}^{-1}$

Figure 41 shows some important behavior via the mole fraction profiles that will occur with this H_2 vitiation. Hydrogen is more reactive than methane and has no carbon component, so when it reacts it should yield H radicals. The vitiated case shows by comparison that this is occurring as the mole fraction of the yielded H radical is over one order of magnitude higher than in the pure nitrogen hot stream case. Since there are greater levels of H radical and an active fuel species, H_2 , in the hot stream, there will be greater consumption of the diffused oxygen, which is reflected in the profiles as the vitiated case reduces quicker up the hot stream and in Figure 42 which shows the larger

consumption rate of O_2 by the vitiated case across the domain. The H_2 vitiation is essentially addition of a fuel, so the greater degree of consumption of oxygen is expected; a catalytic igniter that generates products from a fuel rich flow through the catalytic tube will be expected to have a similar behavior as there will be a similar increase of fuel component, even if some of those components are already broken into radicals and/or partially oxidized.

Figure 42: O_2 Consumption Rate Profiles for .5 Mole Fraction H_2 Vitiated Case and Pure N_2 for $\phi_F = 1.0$, $P = 1$ atm, and $a = 300$ s $^{-1}$

While the maximums of the vitiated species give an idea of what the trends will be, the overall magnitude and behavior of the effect introduced by a vitiated species may be much smaller at the level that it may appear in a combined effect. In order to study the individual effects at the appropriate level, trials were run and examined for each species at a matching concentration. Figure 43 shows the effects of the enhancing species on

ignition temperature by plotting the temperature profiles from the hot stream boundary, exhibiting the ignition temperature, through the ignition kernel. The effect of the molecular hydrogen, with its reduction in ignition temperature from the 1695 K of the pure N_2 case to the 1117 K with vitiation, appears to be much greater than the other species. The other species, at their appropriate levels, seem to have little effect on their respective ignition temperatures, indicating that their individual contribution may be minimal though the cumulative interaction of these species may alter the behavior.

Figure 43: Comparison of Temperature Profiles at the Ignition Turning Point for Different Individual Enhancing Species Vitiation when $P = 1$ atm, and $a = 300 \text{ s}^{-1}$ vs. $\phi_F = 1.0$

While all of these other species have minimal effect on the ignition temperature, oxygen seems to have a slightly different profile in the trend. It is unique in the vitiated species as it is not a radical, fuel, nor product, whereas there are multiple components for

each of those other categories. Though some shifting occurred numerically, there still appears some difference.

Figure 44: Comparison of H Radical Mole Fraction and O₂ Consumption Rate Profiles at the Ignition Turning Point for the cases of Pure N₂ and 1E-3 O₂ Mole Fraction Vitiated Counterflow with P = 1 atm, and a = 300 s⁻¹ vs. $\phi_F = 1.0$

Figure 44 shows how the profiles differ with the addition of the oxygen vitiation. Though the magnitudes of H radical peaks were similar for both trials, the diffusion up the hot stream exhibits some of the effects of this type of vitiation. While there should always be some diffusion of H radical through the ignition kernel into the hot stream, and the trends at first appear similar, the concentration of the H radical falls off to a greater degree in the vitiated trials. Other radicals that diffuse through the kernel also display this trend. Because of the diffusion of radicals, there is some reaction and consumption in the hot stream. The profile of the O₂ consumption rate confirms this as the pure case goes to

zero yet there is a notably higher value with the vitiation. The diffused radicals react with the incoming O_2 causing their consumption and the degradation of some O_2 prior to the ignition kernel. Though these effects can be seen in comparison of the mole fraction and reaction profiles, the overall effect on the ignition temperature for this concentration of O_2 was minimal. This may play a part in a full catalytic ignition system, although the concentration of the radicals should be dominated by those introduced from the catalyst as opposed to having diffused through the kernel.

Figure 45: Comparison of Temperature Profiles for Individual Vitiation of Inhibiting Species with $\phi_F = 1.0$, $P = 1$ atm, and $a = 300 \text{ s}^{-1}$

Figure 45 shows the individual effects of the three retarding species at their respective mole fraction vitiations. While water and carbon dioxide show a small rise in

ignition temperature due to their dilution, they are stable products of combustion and will have minimal chemical effect. The methane behavior is different however, showing a perpetual decrease in the temperature profile throughout the hot stream domain as opposed to the relatively constant temperature of the hot stream in the other cases.

Figure 46: Heat Release Rate Profiles of Counterflow Ignition at Ignition Turning Point for a .1 Mole Fraction CH_4 Vitiated Case for $\phi_F = 1.0$, $P = 1 \text{ atm}$, and $a = 300 \text{ s}^{-1}$
Note: Positive is Endothermic

Figure 46 shows the heat profile of this methane vitiated case. It can be seen that in the hot stream, it is entirely endothermic, positive, up until the ignition kernel. In order to determine which reactions are causing this endothermic temperature decrease, the point of maximum heat consumption rate in the hot stream was determined and those reactions with the greatest heat consumption rates are listed below in Table 6.

Reaction #	Corresponding Reaction Formulation	Heat Release Rate ergs/sec*cm ³
-52	CH ₄ (+M) <=> H+CH ₃ (+M)	2.27E+07
-71	C ₂ H ₃ (+M) <=> H+C ₂ H ₂ (+M)	1.00E+07
-74	C ₂ H ₅ (+M) <=> H+C ₂ H ₄ (+M)	3.66E+07
159	2CH ₃ <=> H+C ₂ H ₅	9.94E+06
174	C ₂ H ₄ (+M) <=> H ₂ +C ₂ H ₂ (+M)	5.12E+06

Table 6: Endothermic 1E-1 Methane Vitiation Hot Stream Reactions at Maximum Endothermic Point in Hot Stream at the Ignition Turning point for P = 1 atm, and a = 300 s⁻¹ vs. $\phi_F = 1.0$
Note: Positive is Endothermic

These reactions show that the methane is breaking down thermally, by the reaction -52, and the resulting CH₃ continues on to be recombined into larger hydrocarbons that also continue to break down and yield more H radicals and H₂. While there are many reactions involved to various degrees, these are all endothermic steps and the overall trending consumes methane endothermically so that the temperature drops prior to the ignition kernel. Because of this fact, there needs to be a higher boundary temperature so that there is enough thermal energy remaining after the hot stream reactions so to cause ignition. These reactions do yield some radicals which may help ignition, but enough methane survives to interfere with the ignition kernel, causing it to be richer than with the pure N₂ case, requiring a higher ignition temperature.

5.5: Combined Effects of Catalytic Igniter

The cases that were chosen to run for the primary full catalytic igniter in counterflow trial started at 1 atmosphere and proceeded up to 100 atm. Rather than matching the catalytic output from PLUG trials at the same given pressure, a single case was chosen as defined before that had a typical consistency of the major species. The

cold flow mixture to be ignited was chosen with an equivalence ratio of $\phi = 1$. Further variation of equivalence ratio will have to be carried out in order to properly characterize ignition capability. In an application of an ignition system such as this, even though the overall mixture could be from stoichiometric to a given fuel rich mixture, stratification in mixture composition may be present. As shown previously, however, the magnitude of temperature variation with equivalence ratio was much smaller than the possible temperature variation achieved through catalytic vitiation.

The strain rate is set at $a = 300 \text{ s}^{-1}$; another worst case scenario when referencing the required ignition temperature comparison done previously. If the incoming catalytically reacted flow is shown to react significantly before reaching the ignition kernel further study should be done with this variation as this would affect the velocity and therefore residence time. While further radical generation may aid ignition, more stable products may also be produced, hindering it.

Figure 47: Ignition response Curve for Combined Catalytic Igniter Trial Cases
 $\phi=1.0$ and $a = 300 \text{ s}^{-1}$
Note: Solid Symbols are the Ignition Turning Points

Figure 47 shows the computed ignition response curves for combined catalytic igniter cases as a function of pressure. While the temperature at the 1 atm turning point is not as low as the H_2 vitiated case, it is less than the pure N_2 case, showing a distinctive advantage for using a catalytic inlet condition. In terms of practical usage of a catalytic igniter, the temperature that is required for ignition is 1228 K, much less than the yielded temperature result from the plug trial of 1520 K. This indicates that under these conditions, the catalytic igniter would be capable of initiating ignition in a counterflow configuration.

The figure also shows that with rising pressure, there is initially a large decrease in the ignition temperature with a rise in the kernel radical mole fractions as the pressure aids ignition as it did without vitiation. The mole fraction concentration of the H_2O_2 tends to level out as the pressure increases with minimal changes even though the ignition temperature keeps decreasing.

Figure 48: Ignition and Maximum Temperatures for Catalytically Vitiated Counterflow Ignition as a Function of Pressure $\phi=1.0$ and $a = 300 \text{ s}^{-1}$

In plotting the trend of the required ignition temperature as a function of the pressure, Figure 48, it is seen that initially at lower pressures, there is a linear decrease of ignition temperature with the log of rising pressure. This linearity falls off however at

higher pressure. Once again, it can be seen that there is a separation of the ignition and maximum temperatures as exothermicity comes into play. Since there is a heat release, not all of the ignition energy needs come in from the hot stream, some comes from the reaction. The data gives rise to this as it can be seen that at first the ignition temperature is below the linear trending and the maximum is above it. As the pressure continues to rise, this effect is similar, though even the ignition temperature rises above the initial linear trending, the exothermicity effect due to chemical energy isn't as effective, and more thermal energy via a higher initial hot stream temperature is required to overcome the chain termination reactions that grow in importance.

In examining the temperature profiles, Figure 49, both cases selected show that they generally follow similar trends to their non-vitiated counterparts, getting thinner as the pressure rises. Likewise, since some of the components that were introduced in the hot stream were reactive, both cases exhibit some exothermic behavior and temperature rise. The 1 atm case rise is very slight, though the 100 atm case rise is more pronounced and has a peak in the reaction zone. The reduction in ignition temperature with increasing pressure is not as significant with the catalytic boundary condition. Comparing Figure 49 with Figure 33, using the catalytic igniter at 1 atm would result in over a 450 degree K decrease in required ignition temperature over the heated nitrogen case. At 100 atm, the benefit is only a little over a 300 degree K improvement.

Figure 49: Temperature Profiles of 1 atm and 100 atm Catalytic Boundary Cases
 $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

Examining the profiles of the components introduced give the first indication of how this behavior occurred. Figure 50 shows the major products at 1 atm. The H_2 , O_2 , and CH_4 show non-peaked profiles. This is expected for the O_2 and CH_4 but without vitiation, H_2 has a peak, but once again, the amount of it in the hot stream overrides the generation at the kernel. CO and H_2O show small peaks in the kernel region so there is some significant generation present.

Figure 50: Major Components for Catalytic Boundary Case at 1 atm, $\phi_F = 1.0$, and $a = 300 \text{ s}^{-1}$

In terms of the minor components as seen in Figure 51, from the start of the hot stream at the rightmost boundary, there is some noticeable decrease in CH_3 and H . There is some generation of C_2H_6 , which rises to greater than ppm concentration ahead of the reaction zone. While the CH_3 to C_2H_6 relationship can be explained through simple recombination, the consumption of the H radical would not be a participant in this reaction, so there must be additional chemistry occurring.

Figure 51: Minor Components for Catalytic Boundary Case at 1 atm,
 $\phi_F = 1.0$, and $a = 300 \text{ s}^{-1}$

Examining a point in the hot stream away from both the boundary and ignition kernel will determine the upstream chemistry that causes the change in composition prior to the ignition kernel. The location to be examined will be at 1.395 cm, where there is the local peak in temperature, though the peak is only about a tenth of a degree rise over the boundary temperature. The reaction rates of progress will give an idea which reactions are responsible for these changes.

Reaction #	Corresponding Reaction Formulation	Reaction Rate of Progress moles/sec*cm ³
84	$\text{OH} + \text{H}_2 \rightleftharpoons \text{H} + \text{H}_2\text{O}$	8.38002E-08
53	$\text{H} + \text{CH}_4 \rightleftharpoons \text{CH}_3 + \text{H}_2$	4.32913E-08
38	$\text{H} + \text{O}_2 \rightleftharpoons \text{O} + \text{OH}$	4.22213E-08
3	$\text{O} + \text{H}_2 \rightleftharpoons \text{H} + \text{OH}$	3.04303E-08
158	$2\text{CH}_3(+\text{M}) \rightleftharpoons \text{C}_2\text{H}_6(+\text{M})$	2.39584E-08
52	$\text{H} + \text{CH}_3(+\text{M}) \rightleftharpoons \text{CH}_4(+\text{M})$	2.33608E-08
98	$\text{OH} + \text{CH}_4 \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$	1.67437E-08
120	$\text{HO}_2 + \text{CO} \rightleftharpoons \text{OH} + \text{CO}_2$	1.35917E-08
11	$\text{O} + \text{CH}_4 \rightleftharpoons \text{OH} + \text{CH}_3$	1.20559E-08
33	$\text{H} + \text{O}_2 + \text{M} \rightleftharpoons \text{HO}_2 + \text{M}$	1.11751E-08

Table 7: Reactions with Greatest Reaction Rate of Progress in Hot Stream at Local Temperature Peak in Catalytic Igniter Case at 1 atm

These reactions are those that had a reaction rate of progress of greater than 1E-8. While other reactions will exist and contribute, they will be to a lesser extent. With the results of the profile and the reaction rates of progress, it can be seen that the change in the CH₃ mole fraction is due to it being consumed in recombination as thought, both to CH₄ and C₂H₆. It is also created by two other reactions, numbers 98 and 11, so some of the consumption effect is nullified, resulting in the small change seen. H is both consumed and produced in a variety of pathways, with the resulting net change being slightly negative. Even though some of the more major components such as methane and H₂ are consumed to a comparatively large degree when comparing to the minor products, their concentrations are so much greater that the resulting change is minimal. It should be noted that the rate of progress of these reactions are about three orders of magnitude

greater in the ignition kernel. Though the level is smaller upstream and other reactions would be more active in the kernel, these aren't negligible as they did have some effect on the composition of the hot stream, most noticeably the approximately two order of magnitude change in C_2H_6 .

In the ignition kernel, setting an absolute threshold cutoff in heat release determines the most important reactions for analysis. Here, it will be carried out at the point of maximum heat release at 1.01 cm. Though this case did not show a large exothermic temperature peak, there is a degree of exothermicity, it just is along the temperature gradient so no peaking occurs. Though these reactions are determined at one location, these reactions should be participants throughout the kernel, only the relative importance may vary. An absolute threshold of $1E+7$ ergs/sec*cm³ was set, so as to capture the major endothermic and exothermic reactions in order to compare their effects. These are as follows in Table 8.

At the ignition kernel, propagation and branching reactions are the majority of the equations. There are a few reactions that yield final products, primarily water as the carbon dioxide producing reactions are found to be less involved in this case. Many of the reactions here in the ignition kernel are similar to those that were in the hot stream though there are some additional reactions that are noted now. HO_2 chemistry has been enhanced, as has chemistry involving larger hydrocarbon radicals such as CH_3O and CH_2O . Additionally, there is more of a presence of O_2 involved reactions as in the counterflow ignition kernel than in the hot stream. There will be more O_2 available via diffusion into the kernel whereas the hot stream had less oxygen involvement because the

initial mixture through the catalyst is very fuel rich and much of that oxygen had been reacted within the platinum tube and was not vented out.

Reaction #	Corresponding Reaction Formulation	Heat Release Rate ergs/sec*cm ³
Exothermic		
84	$\text{OH}+\text{H}_2\rightleftharpoons\text{H}+\text{H}_2\text{O}$	-6.14E+07
158	$2\text{CH}_3(+\text{M})\rightleftharpoons\text{C}_2\text{H}_6(+\text{M})$	-5.20E+07
119	$\text{HO}_2+\text{CH}_3\rightleftharpoons\text{OH}+\text{CH}_3\text{O}$	-4.54E+07
52	$\text{H}+\text{CH}_3(+\text{M})\rightleftharpoons\text{CH}_4(+\text{M})$	-4.48E+07
33	$\text{H}+\text{O}_2+\text{M}\rightleftharpoons\text{HO}_2+\text{M}$	-4.22E+07
168	$\text{HCO}+\text{O}_2\rightleftharpoons\text{HO}_2+\text{CO}$	-3.72E+07
98	$\text{OH}+\text{CH}_4\rightleftharpoons\text{CH}_3+\text{H}_2\text{O}$	-2.24E+07
46	$\text{H}+\text{HO}_2\rightleftharpoons 2\text{OH}$	-1.92E+07
120	$\text{HO}_2+\text{CO}\rightleftharpoons\text{OH}+\text{CO}_2$	-1.77E+07
58	$\text{H}+\text{CH}_2\text{O}\rightleftharpoons\text{HCO}+\text{H}_2$	-1.55E+07
35	$\text{H}+\text{O}_2+\text{H}_2\text{O}\rightleftharpoons\text{HO}_2+\text{H}_2\text{O}$	-1.43E+07
45	$\text{H}+\text{HO}_2\rightleftharpoons\text{O}_2+\text{H}_2$	-1.26E+07
169	$\text{CH}_2\text{OH}+\text{O}_2\rightleftharpoons\text{HO}_2+\text{CH}_2\text{O}$	-1.01E+07
Endothermic		
38	$\text{H}+\text{O}_2\rightleftharpoons\text{O}+\text{OH}$	2.31E+07
-57	$\text{CH}_3\text{O}(+\text{M})\rightleftharpoons\text{H}+\text{CH}_2\text{O}(+\text{M})$	1.98E+07

Table 8: Reactions with Greatest Heat Consumption Rate at the Ignition Kernel Heat Release Peak in Catalytic Igniter Case at 1 atm
Note: Positive is Endothermic

At 100 atmospheres, Figure 52 shows that the mole fraction profiles of the major species have quite similar trends through the domain as they did in the 1 atmosphere trial,

save for the fact that the narrowing with pressure occurred as it did in the pure nitrogen ignition case.

Figure 52: Major Components for Catalytic Boundary Case at 100 atm
 $\phi_F = 1.0$, and $a = 300 \text{ s}^{-1}$

The minor species profiles shown in Figure 53 show quite a difference from the 1 atm case profiles. The profiles show a large amount of composition change near to the hot stream inlet. The reason that this occurs is that for a basis of comparison, a select number of species was chosen for the catalytic inlet based on one output profile from PLUG. The 100 atm results from PLUG had more species with greater than ppm level concentrations, though they all have relatively very small concentrations, as the generated species at the boundary also showed. These species tended to be the larger recombined species that are formed as a result of high pressure. As seen in the minor species profile, what happens near the inlet is the generation of some of these larger species. Even though it appears that there is a great deal of change in some concentration magnitudes it is only in the minor species at very small levels. There was no major effect shown in the

temperature plot near to the inlet in Figure 49 nor were there any inconsistencies at the boundary as shown in the heat release graph, Figure 54. These pressure-compensating changes all go to completion far away from the ignition kernel so that these boundary effects will not cause any errors in the ignition kernel. By including the matched PLUG output from a 100 atm case as the mass fraction inputs, the profiles may be smoother appearing, but there will still be some change near to the inlet as there are different diffusion constraints, no surface chemistry, and a much different temperature. The catalytic output temperature was at least around 600 degrees Kelvin higher than what the calculated hot stream temperature would be required to be. While this is beneficial to obtaining ignition, the profiles we may try to use as the boundary condition may not be supported by a lower required temperature and will undergo such a change near the inlet.

Figure 53: Minor Components for Catalytic Boundary Case at 100 atm
with $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

**Figure 54: Heat Release Profile for Catalytic Boundary Case at 100 atm
with $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$
Note: Positive is Endothermic**

Away from the inlet, but upstream from the ignition kernel, there are noted variations of the minor species. Though many species change, most stay near to their order of magnitude. As the figure indicated, there are some species that grow or are consumed to a high extent prior to the ignition kernel. In examining the heat release profile through the domain, Figure 54, it is seen that there is a peak in heat release, where positive is exothermic for this case, in the hot stream. In order to determine what the primary controlling reactions are for this behavior and the interaction in the hot stream, the individual heat releases for the reactions will be evaluated. Those that had the greatest values, above an absolute threshold of $1\text{E}+8 \text{ ergs/sec*cm}^3$, are in Table 9.

Reaction #	Corresponding Reaction Formulation	Heat Release Rate ergs/sec*cm ³
Exothermic		
120	HO₂+CO<=>OH+CO₂	-2.75E+09
168	HCO+O₂<=>HO₂+CO	-1.16E+09
33	H+O₂+M<=>HO₂+M	-1.05E+09
84	OH+H₂<=>H+H₂O	-6.90E+08
-167	H+CO+M <=> HCO+M	-5.43E+08
35	H+O₂+H₂O<=>HO₂+H₂O	-2.17E+08
98	OH+CH₄<=>CH₃+H₂O	-1.27E+08
99	OH+CO<=>H+CO₂	-1.05E+08
Endothermic		
-85	H₂O₂(+M) <=> 2OH(+M)	1.45E+08

**Table 9: Greatest Heat Contributing Reactions at
Heat Release Peak in Hot Stream for Catalytic Igniter Case at 100 atm
Note: Positive is Endothermic**

What these results yield is that the major heat contributing, and sapping, reactions at this pressure are somewhat different than at the lower pressure. The reactions involving the heat release for this region have greater importance on OH and HO₂ chemistry. The only endothermic reaction that met the set threshold value is a branching reaction that produces further OH and only consumed one percent of the total heat release. Additionally of note is that the two reactions with the greatest heat release follow each other; the products from the second greatest are the direct reactants in the greatest, a linear exothermic pathway that will yield a third of the total release. The majority of these reactions also result in the formation of stable products of combustion, termination

reactions. They may be exothermic, which will aid ignition, but will sap some of the radical pool in the process and deliver inert products to the ignition kernel.

Figure 55: Ignition Kernel View of Minor Components for Catalytic Boundary Case at 100 atm with $\phi_F = 1.0$ and $a = 300 \text{ s}^{-1}$

It has already been seen that there were different reactions in the hot stream at different pressures and the composition of the species being delivered to the ignition kernel is different under these conditions. The different composition of the gas entering the ignition kernel, as well as the different pressure and local temperature, should change the ignition kernel chemistry significantly. Figure 55 shows the minor species mole fractions in the ignition kernel under these conditions. While it was shown that the major species exhibited similar trends, save for the thinning, these minor species trends are somewhat different. Radicals that had dominant concentrations, like H radical and CH_3 , are now in the minority.

One of the visible differences between the 1 and 100 atm cases is that the 100 atm case exhibited a local temperature peak. In order to characterize the ignition chemistry in the kernel and examine this behavior, the individual heat releases for the reactions will be evaluated at the point of maximum heat release within the ignition kernel. Those that had the greatest values, above an absolute threshold of $1\text{E}+8 \text{ ergs/sec}\cdot\text{cm}^3$ are shown below.

Reaction #	Corresponding Reaction Formulation	Heat Release Rate $\text{ergs/sec}\cdot\text{cm}^3$
Exothermic		
120	$\text{HO}_2+\text{CO}\rightleftharpoons\text{OH}+\text{CO}_2$	-7.93E+09
33	$\text{H}+\text{O}_2+\text{M}\rightleftharpoons\text{HO}_2+\text{M}$	-4.97E+09
84	$\text{OH}+\text{H}_2\rightleftharpoons\text{H}+\text{H}_2\text{O}$	-1.79E+09
168	$\text{HCO}+\text{O}_2\rightleftharpoons\text{HO}_2+\text{CO}$	-1.67E+09
35	$\text{H}+\text{O}_2+\text{H}_2\text{O}\rightleftharpoons\text{HO}_2+\text{H}_2\text{O}$	-1.19E+09
-167	$\text{H}+\text{CO}+\text{M}\rightleftharpoons\text{HCO}+\text{M}$	-7.58E+08
98	$\text{OH}+\text{CH}_4\rightleftharpoons\text{CH}_3+\text{H}_2\text{O}$	-3.91E+08
99	$\text{OH}+\text{CO}\rightleftharpoons\text{H}+\text{CO}_2$	-2.93E+08
116	$2\text{HO}_2\rightleftharpoons\text{O}_2+\text{H}_2\text{O}_2$	-2.52E+08
115	$2\text{HO}_2\rightleftharpoons\text{O}_2+\text{H}_2\text{O}_2$	-1.06E+08
119	$\text{HO}_2+\text{CH}_3\rightleftharpoons\text{OH}+\text{CH}_3\text{O}$	-1.05E+08
Endothermic		
-85	$\text{H}_2\text{O}_2(+\text{M})\rightleftharpoons 2\text{OH}(+\text{M})$	5.15E+08
-47	$\text{HO}_2+\text{H}_2\rightleftharpoons\text{H}+\text{H}_2\text{O}_2$	2.27E+08

**Table 10: Greatest Heat Contributing Reactions at
Heat Release Peak in Ignition Kernel for Catalytic Igniter Case at 100 atm
Note: Reactions 115 and 116 are declared duplicate reactions in GRI-MECH
Note: Positive is Endothermic**

These reactions are similar to those in the hot stream at the same conditions, though in general there is a greater magnitude of heat release or heat consumption in this ignition kernel for a given reaction. Not all magnitudes increase proportionately; the differences in concentration and temperature between the kernel and the upstream region will have compounding effects, changing the production and heat release differently. The difference in magnitudes of heat release was expected as there was only the primary peak in temperature within the ignition kernel at this high pressure case. Comparing the heat release for reactions at 100 atm to that of the same reactions at 1 atm also shows why the peak in temperature occurs; the heat release of some of the reactions are almost two orders of magnitude greater. Though exothermic behavior existed in the hot stream as discussed, it was not quite as large in magnitude as within the kernel as seen in Figure 54.

Because of the greater amount of reaction and larger heat release in general within the kernel, a few additional reactions surpassed the threshold that were not as influential within the hot stream analysis. All of these additional reactions that did pass the threshold, when comparing to the hot stream reactions, had HO_2 chemistry as part of their behavior. When comparing with the atmospheric pressure case, while some reactions are common for both, there are some categorical differences between the low and high pressure. At lower pressure, there were more reactions that dealt directly with the consumption of the methyl radical and more of the featured reactions that reacted H radical with another species. While these reactions are still present to some degree at 100 atmospheres, they do not contribute as much to the behavior. At high pressures, there is more CO chemistry as shown by reaction 99 and -167 which did not have a comparable

magnitude at 1 atm. Likewise, there is a greater importance with HO₂ chemistry as shown by the duplicate reactions 115 and 116 as well as the endothermic reaction -47.

Other than more variation of conditions, in order to better develop these results, the sub-ppm level concentrations could be added back in. While individually they did not demonstrate a large effect, it was seen that C₂H₆, HCO, and HO₂ were produced. Including these would start them at a non-zero concentration so they may rise to concentrations that may cause different results. C₂H₆ reached a concentration that had an effect on ignition in the individual trials and the other two species were seen to be part of the major heat releasing reactions. The expected changes would be small as the individual trials showed that concentrations on their scales had relatively minimal effects.

In summation, for the baseline of heated nitrogen versus a stoichiometric mixture of methane and oxygen at atmospheric pressure with a cold stream temperature of 300 K and a strain rate of 300 s⁻¹, the resulting ignition temperature was 1695 Kelvin. With the catalytic hot stream, the required ignition temperature came down to 1220 Kelvin. This required minimum ignition temperature is lower than the 1500 Kelvin output temperature that corresponded to the same conditions that generated the catalytic concentrations that were used proving that ignition could occur. At 100 atmospheres, the baseline ignition temperature with heated nitrogen was 1240 Kelvin, and with the full catalytic vitiation it was reduced to 930 Kelvin, also lower than the catalytic output temperature. These results show that a concept of a catalytic ignition system is feasible.

Chapter 6: Conclusions and Future Work

The development of a catalytic ignition system would be beneficial to space exploration efforts as it specifically addresses a problem. That issue is the difficulty in igniting methane, the primary fuel that can be produced via in-situ resource utilization on Mars, the current ultimate goal for the United States space exploration efforts in the near future. It also offers a potentially more efficient and redundant system that can be used to ensure the safety of our efforts.

The purpose of this study was to document the behavior of a fundamental configuration of a potential catalytic ignition system. It sought to characterize the methane and oxygen behavior in a tubular catalytic reactor so to determine what the possible range of yield of conditions and concentrations would be. In counterflow, the ignition of premixed methane and oxygen by heated nitrogen was to be documented and the effects of changing the premixture, the strain, and the pressure were to be studied and a baseline established. The individual effects of the vitiation of catalytically created products across the range shown achievable by the PLUG trials into the hot stream were studied so as to document the resulting behavior. Lastly, the cumulative behavior, simulating an actual catalytic ignition system, was studied across a range of pressure in order to determine if such a catalytic system could cause ignition.

Though different conditions may exhibit different chemical, thermal, and diffusive behavior, the possibility exists that a catalytic igniter would be able to cause ignition across the entire span of pressures and other conditions typical of propulsion systems in which such a device could be used. These required ignition temperatures were

all lower than the temperatures that PLUG was able to produce for a catalytic stream across the same conditions.

While these are all idealized systems with inherent error, the effects studied within should hold true and this concept should be realizable. Implementing this technology may prove to be a benefit to the continued exploration of mankind beyond our planet by providing a new means to cause ignition that may help with redundancy, efficiency, or energy conservation.

In order to further the ability to apply this technology, experimental trials to verify and potentially improve on the computational results will be conducted. A variety of studies will be carried out in order to examine this possibility.

Fundamental trials with a controlled counterflow in an isolated high pressure chamber will be conducted at Case Western Reserve University in the Combustion Diagnostics Laboratory. These will be conducted systematically over a variety of conditions and will be analyzed with laser assisted diagnostic methods such as planar laser induced fluorescence in order to confirm and compare the results with the computation modeling presented here.

A torch igniter based on this concept is being designed and will be tested at NASA Glenn Research Center in the Research Combustion Laboratory. Primary trials will seek to establish a torch output and then should this prove possible and feasible, further testing to refine and implement the design in a rocket combustor may be carried out.

Other computational work that can be carried out in this field may pertain to the broadening of conditions. A larger equivalence ratio range study can be carried out in

order to determine performance under atypical conditions. Additionally, lower inlet temperatures on the premixed side that would be more common in a liquid oxygen/methane system may be a point of study. Variation of fuels or catalysts can also be conducted as methane/oxygen may not always be the optimal fuel of choice.

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