A STUDY OF DETONATIONS, DDT AND DEFLAGRATIONS IN HIGH PRESSURE ETHYLENE-NITROUS OXIDE MIXTURES

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This document describes a study on detonations and deflagration-to-detonation transition (DDT) in nitrous oxide mixtures. This work aims at bridging the lack of knowledge regarding detonations in undiluted nitrous oxide mixtures at initial pressures greater than 1 atm. This will ensure a database of detonation properties which could enable the design and development of propulsion systems and prevent explosion hazards.

At this point, it is important to note that nitrous oxide, like any other oxidizer must be treated with the highest respect and is extremely dangerous when handled without proper care. This statement is based on the fact that nitrous oxide can exothermically decompose above 850 K and also in the presence of impurities. The hazardous incidents associated with this behavior of nitrous oxide are highlighted in the references cited in Chapter 2. The results and conclusions of this work indicate higher detonation pressures and larger pressure fluctuations with nitrous oxide as the oxidizer than with oxygen, which suggest highly unstable detonations. Additionally, special care must be taken in selecting pressure regulators, valves and other flow devices to be used with this gas as certain sealing materials in these devices may not be compatible with nitrous oxide. Due to these reasons, anyone pursuing to use nitrous oxide as a propellant must have an intimate understanding of the oxidizer, its combustion properties with different fuels and experience with high-pressure system design to mitigate risks which all strong oxidizers pose.

In addition to the results in this document, it is highly recommended that the reader reviews the long list of references in Chapter 2 prior to working with nitrous oxide. The experimental setup described in Chapter 3 provides some guidance on the design of combustion chambers to study high-pressure detonations and the theoretical calculations included in Chapter 4 illustrates a method to study combustion

properties with nitrous oxide and other oxidizers before experimental investigation. The author welcomes any questions regarding the proper handling of this oxidizer and any suggestions to improve operational standards used in this work.

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SYMBOLS

a	Sound speed
c_{sp}	Sound speed in combustion products
d	Diameter
g	Acceleration due to gravity
h	Enthalpy
m	Experimentally determined constant in Dorofeev model
\dot{m}	Mass flow rate
n	Global reaction order
p	Pressure
t	Time
u	Flow velocity or induced velocity
x	Distance
A_s	Area of cross-section of sonic venturi throat
C^*	Characteristic velocity
C_d	Coefficient of discharge
D	Detonation velocity
E_a	Activation energy
$E_{density}$	Ignition energy density
I_{SP}	Specific impulse
K	Function used for empirical correlation with run-up distance by
	Bollinger et al.
L	Length
Ν	Heated nichrome wire ignition
P	Detonation pressure
Q	Energy addition

R	Specific gas constant
R_u	Universal gas constant
Re	Reynolds number
\mathbf{S}	Spark ignition
S_L	Laminar flame speed
Т	Temperature
U_{fL}	Visible flame velocity
X_d	Dimensionless run-up distance $= L_{DDT}/d$
X_s	Dimensional run-up distance as defined by Dorofeev
α	Numerical factor in exponential flame acceleration relation
β	Experimentally determined constant in Dorofeev model
γ	Ratio of specific heats
Δ_I	Induction length
Δ_R	Reaction length
δ	Pre-compression factor
δ_L	Laminar flame thickness
ϵ	Wall roughness
ε_I	Activation energy governing sensitivity of induction period
λ	Extent of chemical reaction
λ_{\pm}	Slope of C_{\pm} characteristics
μ	Molecular weight
ϕ	Equivalence ratio
ρ	Density
$\dot{\sigma}_{max}$	Maximum thermicity from ZND calculations
$ au_e$	Exothermic pulse time
$ au_i$	Induction time
θ	Expansion ratio
χ	Mole fraction
χ_{Ng}	Stability parameter developed by Ng et al.

ABBREVIATIONS

CJ	Chapman-Jouguet
DARPA	Defense Advanced Research Projects Agency
DDT	Deflagration-to-Detonation Transition
DL	Darrieus-Landau
DLR	Deutsches Zentrum für Luft- und Raumfahrt e.V. or German
	Aerospace Center
EBW	Exploding Bridge Wire
FA	Flame Acceleration
GM	Göring Mischung
HTPB	Hydroxyl Terminated Polybutadiene
ID	Inner diameter
L/d	Length-to-diameter ratio
LED	Light Emitting Diode
Li-Po	Lithium Polymer
NACA	National Advisory Committee for Aeronautics
O/F	Oxidizer-to-fuel ratio
P&ID	Plumbing and instrumentation diagram
(P)LIF	(Planar) Laser Induced Fluorescence
PMT	Photo-Multiplier Tube
SDT	Shock and Detonation Toolbox
TOF	Time of Flight
TTL	Transistor-transistor logic
UV	Ultra-Violet
VI	Virtual Interface
ZND	Zeldovich-von Neumann-Döring

ABSTRACT

Bangalore Venkatesh, Prashanth Ph.D., Purdue University, May 2020. A Study of Detonations, DDT and Deflagrations in High Pressure Ethylene-Nitrous Oxide Mixtures. Major Professor: Sally P. M. Bane.

Nitrous oxide (N_2O) has gained popularity as a unique oxidizer due to its ability to decompose exothermically, producing nitrogen and oxygen. Additionally, there are concerns about the safety of nitrous oxide in the nuclear industry where it has been observed that stored nuclear waste generates and retains large amounts of flammable gases such as hydrogen and ammonia along with nitrous oxide. These gases are at risk of explosion even in the presence of a weak ignition source which can result in detonations more violent than those initiated directly. Nitrous oxide is also finding an application in the geothermal industry where it is being tested in combination with ethylene as a stimulant mixture to fracture rock. The detonations initiated in this mixture have the ability to produced a network of fractures in the rock formation. In the rocket industry, nitrous oxide has been used for propulsion in multiple systems, but never in a detonative mode. In order to use nitrous oxide in these areas, its detonation properties in combination with a fuel require quantification. Available literature on nitrous oxide-hydrocarbon detonations is mainly restricted to initial pressures below one atm or with dilution. Therefore, detonations with nitrous oxide as the oxidizer are far from being completely characterized. In addition to this lack of general knowledge, understanding of nitrous oxide-fuel detonations at higher pressures, more typical of practical combustion systems is either extremely limited or non-existent.

In the current work, the flame acceleration, deflagration-to-detonation transition (DDT), and detonation properties of a bipropellant mixture of ethylene (C_2H_4) and N_2O are studied as a function of initial pressures. These properties are compared to

those in mixtures of ethylene-oxygen (O₂). These detonations are investigated in a combustion tube designed and fabricated in-house. The performances of these two mixtures are also investigated using theoretical Chapman-Jouguet detonation calculations as a basis of comparison with the measured properties. Additionally, detonation properties in a mixture of acetylene (C₂H₂) and nitrous oxide are also investigated to compare the two fuels. While C₂H₂ is a highly energetic fuel with theoretically high performance, it presents serious practical storage concerns when considered for propulsion applications. These practical issues motivates the investigation of C₂H₄ as a potential alternative fuel, which is relatively easy to manage.

A critical requirement for the application of bipropellant mixtures to detonation systems is rapid flame acceleration to achieve significant chamber pressure rise in a short distance with the potential for a prompt transition to detonation. This DDT behavior of mixtures using N₂O and O₂ with C_2H_4 and C_2H_2 is investigated for increasing initial pressures in the experimental portion of this work. This behavior is quantified by measuring the run-up distances leading to DDT. The pre-compression of the bipropellant mixtures during flame acceleration caused by the accelerating flame is also estimated and directly measured using appropriate instrumentation. These direct measurements of pre-compression are further used to estimate the path of the accelerating flame in the combustion tube. These estimates are compared with the flame tracked by high-speed imaging in an optically accessible combustion tube.

1. INTRODUCTION & BACKGROUND

Detonations have been scientifically observed since the 15^{th} century and studied since the beginning of the 19^{th} century. One of the earliest investigations into this combustion regime was associated with dust explosions in coal mines by Mallard and Le Châtelier [1]. Detonations can originate from explosives, which Lee [2] describes as highly energetic substances with fast reaction rates and can be in gaseous, liquid, or solid form. Upon ignition, chemical reactions can propagate through an explosive at supersonic speeds as a detonation wave, which is a compression shock with an abrupt increase in the thermodynamic state, initiating chemical reactions. Due to the supersonic speeds, the unburned explosive is not affected by the detonation upstream of it. The energy released in the reaction zone behind the shock front supports its propagation and the velocity of the detonation is unsteady. The released energy is converted to internal and kinetic energy of the wave and the self-sustenance of a detonation wave is attributed to the gradients in properties across the wave. The shock front and the reaction zone in a detonation are separated, and this distance between the shock and reaction zone varies depending on whether the detonation is traveling in a medium close to its limits of detonability or in a readily-detonable mixture and on whether it is a gaseous or two-phase medium [3].

Detonations are one of two broad classifications of combustion waves, with deflagrations being the other. A deflagration wave is used to describe all stages of flame development from propagation at the normal laminar burning velocity to the flame-shock complex immediately prior to complete coupling between reaction zone and the shock [3] and transition to detonation. A deflagration wave thus propagates at subsonic velocity relative to the reactant mixture ahead of it. Depending on the conditions, an accelerating flame or deflagration can transition to a detonation. The distance between the ignition location and the point of this deflagration-to-detonation transition (DDT) is referred to as the run-up distance.

Theoretically, detonation waves in gaseous explosives are better understood than those observed in condensed phase medium. This makes it relatively convenient to predict or compare experimental data from detonations involving gaseous reactants with predictions. There are two classical theories which describe detonations: the Chapman-Jouguet (CJ) theory and the Zeldovich, von Neumann and Döring (ZND) theory. These theories are briefly discussed in Sections 1.1 and 1.2 of this chapter as background to the theoretical calculations presented in Chapter 4. Finally, the project organization is outlined at the end of this chapter.

1.1 Chapman-Jouguet (CJ) Theory

The Chapman-Jouguet model (CJ model) is based on the analysis of the conservation equations across a shock wave developed by Rankine and Hugoniot. The original model proposed independently by Champman [4] and Jouget [5] incorporates an energy input term in the traditional Rankine-Hugoniot analysis. For a detonation wave, the transformation of the reactants into products across the wave results in the release of chemical energy. Assuming chemical equilibrium downstream of the wave, the composition of the products can be determined as a function of the thermodynamic state, and thus the chemical energy released across the detonation can be determined [2].

For this analysis, a fixed combustion wave is considered with the reactants entering the wave from the right and leaving towards the left, as shown in Figure 1.1. The initial and final states are defined by the pressure (p), density (ρ) and enthalpy (h)of the flows in these regions and Q is the energy addition per unit mass of the flow behind the shock. The conservation equations of mass, momentum, and energy for one dimensional steady flow across the combustion wave in a shock-fixed coordinate system are given by

$$\rho_0 u_0 = \rho_1 u_1 \tag{1.1}$$

$$p_0 + \rho_0 u_0^2 = p_1 + \rho_1 u_1^2 \tag{1.2}$$

$$h_0 + \frac{u_0^2}{2} + Q = h_1 + \frac{u_1^2}{2} \tag{1.3}$$



Figure 1.1. Initial and final states for the CJ analysis in shock-fixed coordinates. Subscripts 0 and 1 denote reactant and product states, respectively.



Figure 1.2. The tangency or CJ solutions [2]. In this figure only, v on the x-axis is the specific volume or $v = 1/\rho$.

Combining Equations 1.1 and 1.2 gives the Rayleigh line:

$$\rho_0^2 u_0^2 = \frac{p_1 - p_0}{\frac{1}{\rho_0} - \frac{1}{\rho_1}} \tag{1.4}$$

Additionally, Equations 1.1 and 1.2 are used to eliminate the velocity terms in the energy equation, Equation 1.3, and obtain the reaction Hugoniot curve, which represents the locus of downstream conditions for a given upstream or initial condition:

$$\frac{\gamma}{\gamma - 1} \left(\frac{p_1}{\rho_1} - \frac{p_0}{\rho_0} \right) - \frac{1}{2} (p_1 - p_0) \left(\frac{1}{\rho_0} + \frac{1}{\rho_1} \right) = Q \tag{1.5}$$

The condition when the Rayleigh line is tangent to the Hugoniot curve provides two solutions: a minimum-detonation-velocity solution and a maximum-deflagrationvelocity solution. These tangency solutions are referred to as the CJ solutions and are shown in Figure 1.2. At the minimum-detonation-velocity condition, the shock is moving at the CJ detonation velocity, D_{CJ} and the equilibrium state behind the detonation is defined by the CJ detonation pressure (P_{CJ}) , density (ρ_{CJ}) and temperature (T_{CJ}) .

These equilibrium properties are computed by solving the Rayleigh and Hugoniot equations simultaneously for the minimum-detonation-velocity condition, with the assumption that P_{CJ} is much greater than p_0 and that the specific heat ratio does not change between the reactants and products. The solution results in the following expressions:

$$D_{CJ}^2 \approx 2\left(\gamma^2 - 1\right)Q\tag{1.6}$$

$$\frac{P_{CJ}}{p_0} = 1 + \frac{D_{CJ}^2}{(\gamma+1)} \frac{\rho_0}{p_0}$$
(1.7)

$$\frac{\rho_{CJ}}{\rho_0} = \frac{\gamma + 1}{\gamma} \tag{1.8}$$

$$\frac{T_{CJ}}{T_0} \approx \frac{2\gamma\rho_0 Q}{p_0} \left(\frac{\gamma - 1}{\gamma + 1}\right) \tag{1.9}$$

These relations illustrate significant dependencies of the CJ detonation properties on the reactant properties. In particular, the relative trends in measured detonation pressures and estimated detonation velocities from this work can be explained based on these dependencies. The CJ detonation velocity is mainly dependent on the heat of reaction and the ratio of specific heats, which do not vary appreciably with increase in the initial pressure. However, heat of reaction and ratio of specific heats vary as a function of equivalence ratio thereby resulting in a variation of detonation velocity as a function of mixture ratio. The CJ detonation pressure is function of the CJ detonation velocity and the initial density of the reactants. The variations in these theoretical CJ detonation properties for the mixtures considered in this study are presented in Chapter 4 and compared to measurements in Chapter 5.

1.2 Zeldovich, von Neumann and Döring (ZND) Theory

The CJ theory is a purely thermodynamic analysis and neglects any description of the detonation structure, but the detonation structure essentially provides details of the transition processes from reactants to products. The details of the structure provide insight into the propagation mechanism of the detonation wave. Zeldovich, von Neumann and Döring incorporated the well-known concept of ignition via shock compression into their detonation model and described the structure as comprising a leading shock front followed by a chemical reaction zone. Due to the Second World War, the three researchers were unaware of each other's work and so this detonation structure model is now referred to as the Zeldovich-von Neumann-Döring (ZND) model. Zeldovich predominantly studied the effects of heat and momentum losses within this structure on the propagation of the wave and concluded that these losses to the walls result in a detonation velocity less than the equilibrium CJ value. Another conclusion of this theory, based on von Neumann's analysis, is the existence of detonations which have velocities higher than the equilibrium CJ value. In addition to this, Döring concluded that the chemical reaction does not occur immediately behind the shock wave but rather at some non-negligible distance downstream and thus the shock leading the detonation wave can be decoupled from the chemical reactions [2]. This ZND detonation structure can be schematically represented as shown in Figure 1.3.



Figure 1.3. Schematic representation of ZND detonation wave in shock-fixed coordinates. λ represents the extent of chemical reaction. Representation is similar to that in [2].

The ZND theory assumes a unidimensional flow with a leading shock represented by a discontinuity, as in the CJ theory. However, the chemical reaction does not occur directly behind the shock. Instead, the shock is followed by a region where chemically active species are produced at a finite rate at the high temperature and pressure of the shocked medium. The overall chemical reaction is represented by a single forward-rate process, gradually progressing to completion some distance behind the leading shock. This region immediately behind the shock is called the induction zone and is characterized by an induction time τ_i . The assumption is that the overall reaction rate in this region is controlled by a highly endothermic and slow reaction step. This induction time is dependent on the temperature (T_s) and density (ρ_s) of the shocked gas through an Arrhenius expression of the form [3]

$$\tau_i \propto \frac{1}{\rho_s^n} exp\left(\frac{E_a}{RT_s}\right) \tag{1.10}$$

The pressure history associated with the ZND detonation structure includes the von Neumann spike, a region of constant pressure equal to the post-shock pressure (P_s) , where thermoneutral chain-branching reactions occur. This is followed by a region of rapid pressure decrease due to recombination reactions, which culminates

at the CJ plane. Finally, there is a Taylor expansion wave with its head at the CJ plane. This pressure profile is shown in Figure 1.4. However, the constant pressure region (von Neumann spike) is too thin to be resolved even by fast response pressure transducers due to the relatively large size of their sensing surface areas. Therefore, a pressure transducer will only measure a pressure close to and slightly greater than the CJ detonation pressure and as illustrated by curve (b) in Figure 1.4.



Figure 1.4. (a) Idealized ZND pressure profile and (b) experimental profile in $2H_2 + O_2$ mixture at $p_0 = 100$ torr from [3]. τ_i is the induction time and τ_r is the recombination time.

1.3 Project Objective and Organization

In the present work, the use of nitrous oxide and ethylene as a bi-propellant mixture at elevated initial pressures is investigated. Nitrous oxide is an energetic oxidizer which has added benefits such as ease of handling, storability at room temperature, and high vapor pressure. Additionally, ethylene is a stable small chain hydrocarbon, unlike acetylene which has additional energy stored in its double bond. The high vapor pressure of these gases makes them self-pressurizing propellants, thereby improving ease of usage in a rocket engine. It is also known that both nitrous oxide and ethylene are mixable over a wide range of temperatures and have nearly equivalent vapor pressures. This bi-propellant mixture has only recently being investigated in a deflagrative rocket, but their detonations have not yet been investigated. Bipropellants currently being used in detonation rocket engines have been thoroughly characterized in the detonation regime and models exist to predict their performance. Thus, characterizing the detonation properties of ethylene-nitrous oxide will enable the investigation of this energetic mixture for use in detonation engines which are increasing in popularity. This characterization involves accurate measurement of detonation pressure, detonation velocity, cell-width and run-up distance over a range of initial conditions such as initial pressure and temperature, equivalence ratio, ignition energy and dilution.

Literature on nitrous oxide provides detonation properties in combination with fuels such as hydrogen, methane and ammonia. Similarly, literature on ethylene includes detonation experiments and simulations with oxygen and air, which are the most common oxidizers. Most of the previous experimental work is either at sub-atmospheric initial pressures or with nitrogen/argon dilution. Additionally, researchers have developed and improved detailed and reduced chemistry models for nitrous oxide combustion with hydrogen and small hydrocarbons based on shock tube and flame measurements. These chemistry models can then be used to provide a good estimate of ethylene-nitrous oxide combustion properties. Information from ethylene-oxygen detonation experiments provide an order of magnitude assessment of the detonation properties to expect from ethylene-nitrous and the design of the experimental setup for the current project is based on this review. The next chapter in this document details these references and reviews some important studies involving nitrous oxide flames, chemical kinetics, detonations and propulsion systems. It also includes a brief section on flame acceleration and DDT studies. Following this, Chapter 3 describes the design, working and instrumentation of the experimental setup used to study flame acceleration and detonation properties in ethylene-oxidizer mixtures. Next, a discussion on theoretical calculations of detonation and flame properties is included in Chapter 4. The values obtained from CJ detonation calculations are later used for comparison with measurements from experiments. The flame properties are included to help explain run-up distance and flame acceleration trends resulting from experiments. The measured detonation pressures and average velocities from experiments are discussed in Chapter 5 along with comparisons to CJ detonation pressures and velocities. Finally, Chapter 6 presents the estimated run-up distances and pre-compression. The pre-compression is measured using appropriate pressure transducers and is visualized in an optically accessible planar detonation tube.

The main objectives of this project can be summarized as follows:

- 1. Measure detonation pressure, velocity and run-up distance for ethylene-nitrous oxide as a function of initial pressure.
- 2. Measure these properties for ethylene-oxygen in the same experimental setup for one-to-one comparison.
- 3. Compare the performance of ethylene to that of acetylene with nitrous oxide since acetylene is a more energetic fuel, but unstable.
- 4. Investigate the effect of different ignition energies on the run-up distance (2 levels).
- 5. Measure the pre-compression of the unburned gas mixture prior to DDT in order to understand the mixture's behavior in a constant volume combustor.
- 6. Study deflagrations and flame acceleration (FA) in ethylene-nitrous oxide in an optically accessible combustor.

Preliminary work with this bi-propellant mixture at higher initial pressures shows an extremely fast transition to detonation in a short, closed tube 24.5 inches long with a 4 inch inner diameter using a weak ignition source [6]. The results from these earlier tests suggest that a steady detonation can be established in a combustion tube of larger L/d ratio and the associated flame acceleration prior to DDT could be studied more accurately. These preliminary results are discussed in Chapter 5 in detail. This fast transition to detonation involving rapid flame acceleration is an important characteristic for detonation engines. To study the flame acceleration and DDT behavior of undiluted ethylene/nitrous oxide, this mixture is tested in a large L/d (= 68) closed tube by igniting the mixture with two different ignition methods. This project mainly focuses on investigating this bi-propellant mixture over a range of initial pressures above 1 atm and without any dilution.

2. LITERATURE REVIEW & MOTIVATION

The decomposition and combustion properties of nitrous oxide (N_2O) have been studied for nearly a century. Technical interest in nitrous oxide intensified in the 1960s because of the compound's positive heat of formation, resulting in heat release during decomposition. Also, upon complete dissociation the products are pure nitrogen (N_2) and oxygen (O_2) . These characteristics make nitrous oxide a unique oxidizer for combustion systems, and ignited interest in using N₂O in supersonic wind tunnels to increase enthalpy to simulate high speed flight conditions.

This chapter presents a review of past research on this bi-propellant mixture and divides these studies into two categories: 1) detonations and 2) flame acceleration and DDT. Studies on flames involving nitrous oxide and their chemical kinetics and nitrous oxide decomposition are included in the second category.

2.1 Detonations in Mixtures Including Nitrous Oxide

A great deal of work was done by the Air Force in the 1960s to characterize the decomposition and detonability of nitrous oxide at elevated temperatures and pressures. One of their conclusions was that it was difficult to initiate detonation waves in pure nitrous oxide, but explosions from high rates of chemical reaction were observed by Laughrey et al. [7] in 1962. Decades later in 1998, Pfahl et al. [8] also confirmed that it was not possible to achieve detonations in mixtures with less than 5% hydrogen in nitrous oxide. Due to this, future investigations into nitrous oxide detonations involved at least one fuel component. In 1962, Bollinger et al. [9] measured detonation velocities and run-up distances in hydrogen-nitrous oxide mixtures of varying initial pressures and fuel concentrations in a 79 mm ID tube. They ignited the mixtures by melting a thin copper wire using a 28 VDC power supply. Their results showed that at low fuel concentrations the detonation velocity decreased with increasing initial pressure, and vice versa at richer concentrations. They also observed that the runup distances decreased with increasing pressure but appeared to level off at 10 atm pressure.

Later in 1997, there was motivation to quantify the detonation cell widths for N_2O -fuel and O_2 -fuel mixtures as cell size is a metric to assess detonability and can be correlated with the computed reaction zone thickness behind idealized detonation waves. This correlation could then be used to predict cell widths at untested conditions. To this end, researchers at the Explosion Dynamics Laboratory at Caltech used a 11 in. inner diameter, 24 ft. long combustion tube, which was first referenced in 1993 [10], with an oxy-acetylene driver to study detonations close to CJ conditions. Akbar et al. [11] studied detonations in the above oxidizers with H_2 , CH_4 and NH_3 as the fuels with N_2 dilution as another variable. The cell width data for CH_4 - N_2O diluent mixtures they published was new information with no comparable data from other studies. They observed that the average measured wave speeds between consecutive pressure transducers were very similar to the equilibrium detonation speed predictions thereby confirming the accuracy of CJ detonation calculators. They compared cell widths for mixtures without dilution and at an initial pressure of about 1 atm and reported that H_2 and CH_4 have slightly smaller cell widths with O_2 as the oxidizer than with N_2O . The situation was reversed in NH_3 , which had a smaller cell width with N_2O as an oxidizer versus O_2 . They attributed the behavior with NH_3 to the possible existence of a direct channel of reaction that is not present in either H_2 or CH₄. Their correlation of measured cell widths to calculated ZND reaction zone thicknesses resulted in a power law, but different fuel-oxidizer combinations followed different power law exponents. This led the authors of [11] to conclude that a physical theory that would suggest a functional relationship between cell width, reaction zone thickness and other properties of a mixture was a key missing element in achieving a general correlation for all combustible mixtures.

The following year, Pfahl et al. [8] used the same experimental setup as Akbar et al. [11] to measure detonation cell width, velocity and pressure for a range of equivalence ratios in hydrogen-nitrous oxide, with and without 30% nitrogen and/or 50% air dilution at 0.7 atm and 295 K. They also investigated the effect of 3% methane or 3% ammonia addition. The cell width versus concentration curves they obtained for the above mixtures had the familiar U-shape similar to that of hydrocarbon fuels in air. The nitrogen dilution cell widths were larger than those with no dilution and those with additional air dilution were further larger than those with just nitrogen dilution. When they compared cell widths from nitrous oxide mixtures with those using oxygen, they observed some difference. For lean mixtures, cell widths were substantially smaller than in an hydrogen-oxygen-diluent mixture with the same equivalence ratio, and they attributed this reduction to the exothermic decomposing nature of nitrous oxide. For stoichiometric hydrogen-nitrous oxide mixtures, the addition of methane or ammonia resulted in an increase in cell width indicating their role as inhibitors to the base mixture. The effect of nitrous oxide's exothermic decomposition was further discussed by Kaneshige et al. [12]. They stated that detonation velocities of stoichiometric mixtures were higher when oxygen was used as the oxidizer than nitrous oxide due to the dissociation of nitrous oxide generating nitrogen which dilutes the combustion products, thereby offsetting the energy release due to the positive heat of formation of N_2O . However, for fuel-lean mixtures, the energy release from N_2O decomposition can result in a more detonable mixture with nitrous oxide as the oxidizer than with oxygen.

Most of the experimental studies on fuel-nitrous oxide mixtures were conducted at sub-atmospheric initial pressure and the limited high pressure work was restricted to shock tube species measurements. One such work was conducted by Mével et al. [13] in 2007 to investigate the high pressure behavior of induction delay times in H₂-N₂O-Ar mixtures. They discovered that at 9 atm, there was no change in induction delay times for these mixtures with varying temperatures. Using available data, they also developed a correlation between cell width and induction length for H₂-N₂O-N₂ mixtures as a function of equivalence ratio, mole fraction of nitrogen diluent and initial pressure. This correlation agreed well with experimental data from the above mentioned studies at Caltech over the entire range of equivalence ratios from lean to rich. In addition, the shock tube measurements were used to develop a kinetic model for $H_2/N_2O/Ar$ that included excited OH^{*} radicals

Later, Mével et al. [14] experimentally studied detonations in hydrogen-nitrous oxide-argon mixtures over ranges of initial pressures and equivalence ratios and measured the shock velocities and cell widths. They also developed numerical simulations of the detonation front based on a reduced reaction mechanism. An important aspect of this work was their analysis of shock velocity variation within a detonation cell based on numerical calculations. The authors concluded that the leading shock was highly overdriven with normalized velocity as high as $D/D_{CJ} = 1.5$ in the beginning of the cell but dropped to $D/D_{CJ} = 0.8$ at a normalized cell length of 0.8.

From the above discussion, it is not easy to establish detonations in pure nitrous oxide, but its ability to exothermically decompose produces high rates of chemical reactions leading to explosions. The CJ detonation properties of fuel-nitrous oxide mixtures can be predicted using existing calculators with good accuracy and compared well with experimental measurements. The comparable cell widths of mixtures with N_2O and O_2 indicate similar detonability of both these oxidizers when combined with the same fuel. For lean mixtures, the exothermic decomposition nature of nitrous oxide results in comparable or even higher detonability in comparison to oxygen. Several detonation and shock tube studies on hydrogen-nitrous oxide mixtures led to the development of kinetic mechanisms which form the basis for hydrocarbon-nitrous oxide mechanisms. However, there is a gap in fuel-nitrous oxide detonation data at initial pressures above 1 atm without dilution which the current work aims to bridge. In general, it is very difficult to directly initiate detonations in a combustible mixture and so to understand the development of detonations, it is important to study deflagrations and the deflagration-to-detonation transition process. Deflagration-todetonation transition in combustible mixtures is a stochastic phenomenon and many studies have been conducted to understand the mechanisms involved and the influencing factors. In 1883, Mallard and Le Châtelier [1] demonstrated the possibility of both forms of combustion waves existing in the same gaseous mixture when they observed the transition from a deflagration to a detonation using a drum camera. They were among the earliest researchers to suggest that adiabatic compression of the detonation front is the mechanism by which chemical reactions are initiated in the gas mixture [1]. They interpreted the onset of a detonation as an outcome of violent flame vibrations based on their imaging. Generally, it is observed that an unstable, self-propagating deflagration has the tendency to accelerate continuously upon ignition. If the boundary conditions are appropriate, a deflagration will accelerate to a high velocity before abruptly transitioning to a detonation wave.

In their study on detonations in hydrogen-nitrous oxide mixtures, Bollinger et al. [15] observed that the run-up distances they measured decreased with increasing initial pressure, but leveled off as pressure neared 10 atm. They postulated that the laminar burning velocity, degree of turbulence generated by the accelerating flame, and initial pressure directly influence the run-up distance of a mixture. The turbulence generated by the traveling flame was quantified in terms of the Reynolds number due to the flame generated motion, and for fuel-air flames this Reynolds number increased slightly, remained constant, or even decreased with increasing pressure due to the constant laminar burning velocity. However, the laminar burning velocities of hydrogen-nitrous oxide increased with pressure in about the same proportion as did those of hydrogen-oxygen flames, but the latter system had laminar burning velocities over three times higher than those of hydrogen-nitrous oxide mixtures. So the authors

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theorized that the flame generated turbulence of hydrogen-nitrous oxide flames does not increase as much as that for the hydrogen-oxygen flames with increasing pressure. This led to a slower decrease in run-distances with nitrous oxide in comparison to oxygen as pressure increased because the detonation wave formed more quickly when turbulence was present.

Another important work in this area was that of Wu et al. [16] where they studied flame acceleration and DDT of stoichiometric ethylene-oxygen in capillary tubes of 0.5, 1.0 and 2.0 mm diameters. They were the first to observe DDT in microchannels and the critical channel diameter provides an insight into the cell width of the mixture. They used high-speed video to visualize evolution of the visible flame zone when the mixture was ignited with either a hot wire or a spark igniter. A direct conclusion of their work was that DDT was quicker when ignition energy was increased as shown by their results with the two ignition methods. The flame tip velocities they measured in the 1 and 2 mm tubes reached CJ detonation velocity of this mixture. They observed that the flame zone became brighter as it accelerated downstream and finally issued an abrupt burst in brightness when it transitioned to a detonation. The visualized flame zone accelerated quickly to 100 - 300 m/s in under $20\,\mu s$ and they attributed this to the fast laminar flame speed and high expansion ratio of the stoichiometric ethylene-oxygen mixture. This acceleration dissipated at around 50 μ s momentarily, and the flame accelerated again. They concluded that the second acceleration in the flame was due to the stretching of the planar laminar flame to a parabolic shaped flame front. Based on the the Reynolds number of the flow ahead of the flame they concluded that the flow was turbulent and that this influences the transition to detonation. When they tested in the 0.5 mm tube they observed the effects of quenching on flame propagation with some flames transitioning to a detonation and traveling at near CJ detonation velocity, some transitioning to a detonation but failing to propagate, and finally, some accelerating to a constant speed of approximately 1600 m/s. These different behaviors indicated that the size of the tube might have reached the detonation quenching limit for this particular gas mixture.
Other researchers around this time [17–20] also quantified DDT run-up distances by detecting the abrupt burst in brightness during transition by using a photodiode. Moreover, the flame features observed by [16], i.e. two accelerating phases and flame stretching into a tulip structure, were also noted by other researchers [17,21]. In these studies [17,21], the authors also used schlieren visualization to observe compression waves in the flow ahead of the propagating flame.



Figure 2.1. Sequence of shadow photographs show the evolution of the flame front during transition from the first to the second stage. The first frame is taken at 0.5 ms with 0.1 ms between the frames. Hydrogen-oxygen, $p_0 = 0.2$ bar [21].

The experiments and computations conducted by Liberman et al. [21] showed three distinct stages in the flame development prior to DDT: (1) the flame accelerates exponentially producing shock waves far ahead of the flame; (2) the flame acceleration decreases and shocks are formed directly on the flame surface; and (3) the final stage of actual transition to a detonation. They explained that during the first stage the compression waves generated by the accelerating flame steepen to a shock far ahead of the flame at about 67 channel widths. During the second stage the flame acceleration decreases and compression waves steepen to shocks directly at the flame front. Shock waves compress and heat the gases adjacent to the flame front. At this point, a pocket of heated and compressed unreacted gas mixture, called the preheat zone, is formed adjacent to the flame. After this, the flame transitions to a detonation. The formation of the preheat zone ahead of the accelerating flame had been overlooked in previous studies, but the work by Liberman et al. [21] highlighted it as an important feature of the flame dynamics for the mechanism of DDT. This preheat zone and the transition to a detonation were clearly shown in a series of shadow photographs in Figure 2.2. In addition to this, Lee [2] found that investigations of DDT in smooth tubes show that the deflagration accelerates to some maximum velocity on the order of half the CJ detonation velocity of the mixture just before transitioning to a detonation.

The phenomenon of DDT is characterized by a parameter called the run-up distance, which is the distance from the ignition plane to the location of DDT. The above discussed flame acceleration process occurs in this run-up distance and the accelerating flame behaves like an accelerating piston compressing the unburned mixture ahead of it. This leads to the possibility of pressure-piling, a process leading to the production of abnormally high pressures that increase with increasing run-up distances [3]. This process of pressure-piling is further discussed in relation to the measured data in Chapter 5.

Another important feature associated with the transition to a detonation by an accelerating flame is the formation of a shock front and reaction zone traveling back into the products of the flame from the point of transition. This is called the retonation wave. This phenomenon has been captured in observations of DDT as shown in the shadow photograph of a detonation in ethylene-oxygen mixture in Figure 2.2 [21].

Based on these experimental observations and premixed laminar flame theory, various 2D and 3D analytical calculations and numerical simulations of flame acceleration and DDT were developed. Bychkov et al. [22] developed a theory and modeled flame acceleration based on the Shelkin mechanism, which is related to the non-slip wall condition and the increase in flame velocity due to bending of the flame front. They theorized that flames with realistically large expansion ratios accelerate exponentially from a closed end of a tube with nonslip at the walls and that the acceleration is unlimited until a flame triggers detonation. The theory developed by Bychkov et al shows that the velocity profile and the thickness of the boundary layers do not change with distance from the flame in the flow induced by the accelerating flame. Their model predicts acceleration rate as a function of the expansion ratio



Figure 2.2. Series of shadow photographs during flame acceleration and transition to detonation in ethylene-oxygen mixture, $p_0 = 0.12$ bar [21].

the mixture). For large values of Reynolds number, $Re >> 4\theta$, the acceleration rate decreased with increasing Re. While comparing their theory to other mechanisms, Bychkov and coworkers stressed that the velocity increase obtained from their work was much stronger than that provided by the mechanism based on the hydrodynamic Darrieus-Landau (DL) instability of the flame front which is only significant in the very beginning of the acceleration process. In addition, this study was aimed at understanding the flame acceleration in narrow tubes a few millimeters in diameter and the authors concluded that heat transfer to the walls would reduce the flame acceleration actually observed.

Another simplified model of flame acceleration in tubes was developed by Dorofeev [23] based on the hypothesis that the acceleration is directly related to the generation of a turbulent boundary layer in the flow ahead of the flame. As the flame advances in the tube, the flame front propagates with the turbulent velocity in the boundary layer formed ahead of the flame and this is greater than the velocity at the core of the flame. The thickness of the boundary layer ahead of the flame grows with time while the flow interacts with the wall. Based on this model, the author developed an expression for non-dimensional run-up distance, X_s/d , as a function of wall roughness (ϵ), boundary layer thickness and few other experimentally determined parameters (β and m):

$$\frac{X_s}{d} = \frac{\Gamma}{C} \left[\frac{1}{\kappa} ln \left(\Gamma \frac{d}{\epsilon} \right) + K_c \right]$$
(2.1)

$$\Gamma = \left[\frac{c_{sp}}{\beta(\theta-1)^2 S_L} \left(\frac{\delta_L}{d}\right)^{1/3}\right]^{\frac{1}{2m+7/3}}$$
(2.2)

where κ , K_c and C are constants from [17].

In this work run-up distance was defined as the flame propagation distance where the flame speed reached the sound speed in the combustion products. The boundary layer thickness was determined based on the expansion ratio (θ), sound speed in the combustion products (c_{sp}), laminar flame speed (S_L) and laminar flame thickness (δ_L). The model showed good agreement with measurements in H₂-O₂ mixtures with initial pressures less than 1 atm, but deviated above that pressure.

Ivanov et al. [24] developed a model similar to [22] for hydrogen-oxygen flame acceleration and DDT in channels with no-slip. The model was developed based on observations of the propagating flame from earlier experiments by their group [21] where they noted two distant stages. During the first stage of flame propagation, the flame acceleration was related to the stretching of the flame front within the boundary layer, and during the second stage, further fast acceleration of the flame was due to its coupling with the shock wave formed at the flame front. Thus, there were two feedback mechanisms leading to the development of the high flame speed observed prior to DDT, which were incorporated into the model by Ivanov et al. One was driven by the increased temperature, and hence reactivity, of the mixture due to the shock ahead of the flame, and the other by the net increase in the amount of reacting fuel entering the flame front due to increased density. A higher flame speed created a higher gas velocity ahead of the flame. Consequently, the amplitude of the pressure peaks at the flame front continued to grow due to the combustion of the larger amount of compressed mixture entering the reaction zone during the second stage. Eventually, the pressure peak became strong enough to affect reactions. The increase of the reaction rate and the heat released in the reaction zone created a positive feedback coupling between the pressure pulse and the heat released in the reaction, promoting additional flame acceleration. The authors also used high resolution 3D numerical modeling to obtain simulated schlieren and shadowgraph visualizations of the flame acceleration and DDT which matched those from experiments. They provided a three dimensional picture of the flow physics in the flame and ahead of the front.

In summary, studies on flame acceleration and DDT indicate that these phenomena are strongly influenced by properties such as the laminar flame speed and expansion ratio of the combustible mixture. These parameters directly affect the flow induced by the accelerating flame in the unburned mixture ahead of it leading to DDT when the flame accelerates to a critical velocity. One of the developed models theorized that the interaction of the flame with the boundary layer ahead of it creates a turbulent flame in the boundary layer and this mechanism accelerates the flame to critical speeds leading to DDT. Another aspect of flame acceleration leading to detonation is the outcome of detonation pressures and velocities in excess of CJ predictions, which poses a higher rise than directly initiated detonations. The current work also explores this property of nitrous oxide detonations.

2.2.1 Flames in Mixtures Including Nitrous Oxide

As described in the previous section, it is well established that the phenomenon of DDT is dependent on flame properties. This section summaries previous studies on the properties of flames with nitrous oxide as a component. An in-depth comparison of stoichiometric CH_4 -N₂O-Ar and CH_4 -O₂-Ar flame structures was conducted by Vandooren et. al. [25] using molecular beam sampling and mass spectrometric analysis. They observed that the N₂O flame stabilized 2 mm higher above the burner than the O₂ flame and proposed that this displacement in flame front location was due to the lower laminar burning velocity of the flame with N₂O as the oxidizer. Due to this difference in flame front location, they measured lower temperatures near the burner for the CH₄-N₂O-Ar flame. They also noted that both flames had similar thicknesses of about 2.5 mm.

Later, Powell et al. [26] studied mixtures of different fuels with diluted nitrous oxide to determine laminar flame speeds at 0.8 atm. using a flat flame method and compared their results with those calculated using three different chemical kinetic mechanisms. The nitrogen dilution they used was such that $N_2O/(N_2O + N_2)=0.42$ for methane, acetylene and propane, and 0.27 for hydrogen. The laminar flame speeds they measured with acetylene were higher than those measured with methane and propane for the entire equivalence ratio range considered in the study, with a peak flame speed of 48.9 cm/s occurring at $\phi = 1.41$. This flame speed is significantly lower than the peak laminar flame speeds measured for acetylene-air (165 cm/s) [27] and acetylene-oxygen (550 cm/s) [28]. Furthermore, the authors of [26] compared their measured acetylene-nitrous oxide laminar flame speed to that measured by Parker and Wolfhard [29], who studied the characteristics of premixed gas flames of various fuels burning with NO and NO₂. For comparison, Parker and Wolfhard also measured the laminar flame speeds of undiluted fuel- N_2O mixtures and reported a speed of 170 cm/s for acetylene-N₂O. When Powell et al. [26] extrapolated their diluted mixture results to an undiluted condition and compared them with those from |29|, they corresponded closely with the differences being within 14-20 cm/s (8 - 11%) at the equivalence ratios examined.

Upon comparison of experimental and numerical results, Powell et al. [26] observed that the numerical results under-predicted their measurements for both hydrogenand hydrocarbon-nitrous oxide flames. The similarity in laminar flame speed versus equivalence ratio trends of hydrogen and hydrocarbon flames was significant in pointing to the importance of H_2/N_2O reactions to the overall hydrocarbon mechanism and the requirement for more accurate rate constant definitions for the H_2-N_2O sub-mechanism. Based on their measurements of the $H_2-N_2O-N_2$ flame, they modified the reaction mechanism which resulted in better agreement between numerical and experimental flame speed data. In spite of the new rate constants, the flame speeds for methane- and propane-nitrous oxide were still somewhat under-predicted for fuel-lean conditions and over-predicted for fuel-rich conditions. The authors concluded that the deviation in the fuel-rich regime could be reduced by the inclusion of chemistry involving N_2H_x/NH_x species. They explained that the N_2H_x reaction steps act to inhibit the overall H_2/N_2O reaction rate, especially for the fuel-rich cases, and showed that this was predominately due to the recombination reaction producing the hydrazyl radical,

$$NH + NH_2 + M \longrightarrow N_2H_3 + M \tag{R1}$$

In another work, Powell et al. [30] further studied the chemical kinetics of hydrogen and small chain hydrocarbons with nitrous oxide in flames and shock tubes. Their findings about the N_2H_x/NH_x reactions were consistent with those in the $H_2-N_2O-N_2$ flow reactor work by Allen et al. [31] at 3 atm and 995 K. Allen et al. had also found that inclusion of N_2H_x chemistry significantly reduced the predicted overall reaction rate, and thus was necessary to bring their calculations in agreement with measured species profiles.

Bane et al. [32] measured the laminar burning speeds of undiluted and nitrogen diluted H_2 - N_2O mixtures at initial pressures in the range of 20-80 kPa and observed laminar burning speeds as high as 350 cm/s with highly unstable flames. Further, their calculations using a detailed chemical mechanism predicted burning speeds for higher pressures (100-300 kPa) for different H_2 - N_2O mixture ratios. They concluded that the high laminar burning speeds in combination with large expansion ratios (on the order of 10 or higher) and fast onset of cellular instability in these mixtures indicated a hazard of flame acceleration and deflagration-to-detonation transition in H₂-N₂O mixtures. The addition of argon ($\chi_{Ar} = 0.6$) to this mixture by Mével et al. [33] drastically reduced the laminar flame speed they measured in a spherical bomb at 1 atm and 300 K. They measured a peak laminar speed of 56 cm/s for the stoichiometric mixture, which was much lower than that for a mixture of hydrogen-air of around 200 cm/s at the same initial conditions. They attributed this to the difference in the mixture molar mass and the kinetic nature of energy release between the two systems. Under stoichiometric conditions, the molar mass of a hydrogen-air mixture, which limited the flame speed of H₂-N₂O-Ar mixtures. Furthermore, the energy release in H₂-N₂O-Ar mixtures was driven by a linear chain process, whereas in H₂-air mixtures, it was driven by a chain branching process. Consequently, the energy release rate in H₂-N₂O mixtures was slower than in H₂-air mixtures.

Another important work with H₂-N₂O mixtures was an experimental study of minimum ignition energy of lean mixtures [34]. The authors stated that the minimum ignition energy is a function of laminar flame speed and initial pressure. However, based on the observations by Bane et al. [32], the laminar burning speed of H₂-N₂O is independent of pressure over a large range. Thus, the authors of [34] concluded that for a given composition, the ignition energy density is independent of the laminar flame speed and approximately scales with pressure as $E_{density} \sim p^{-1}$. This dependence on pressure was exhibited by their experimental measurements. They also predicted an ignition energy density of less than $1 \,\mu J/mm$ for a stoichiometric H₂-N₂O at an initial pressure of 100 kPa which was comparable to or less than the ignition energy density of H₂-O₂, which was about $5 - 10 \,\mu J/mm$, at similar conditions [35].

The studies described in this section have contributed to improved models and mechanisms to predict thermodynamic and chemical properties in combustible mixtures including nitrous oxide. In addition to this, they have compared nitrous oxide with more traditional oxidizers, like oxygen and air, either to assess the hazard posed by its combustion with different fuels or to understand general nitrogen chemistry in combustion. In comparison to oxygen-fuel mixtures, the peak laminar flame speeds of nitrous oxide-fuel mixtures were lower and this was attributed to the fast chemistry in oxygen flames. However, nitrous oxide laminar flames were either faster or comparable to those with air as the oxidizer. Since laminar flame speed is an important parameter which affects flame acceleration leading to DDT, these speeds will be compared and discussed in Chapter 4. Accurate measurements of laminar flame speeds are critical for better prediction of visible flame velocities used to bridge the gap between flames and detonations using analytical or numerical models.

2.2.2 Chemical Kinetics of Fuel/Oxidizer Mixtures Involving Nitrous Oxide

A logical following discussion is on the chemical kinetics involved in fuel-nitrous oxide systems. Flame velocities, detonation pressures and detonation velocities are some macroscopic properties of combustion regimes. The temporal rate of change of these macroscopic properties are determined by the combustion wave structure, which is controlled by the chemical kinetics associated with the particular fuel-oxidizer mixture and the combustion regime under consideration.

One of the earliest studies on the chemical kinetics of mixtures with nitrous oxide was done by Henrici and Bauer [36] in 1969. The concentration profiles of OH and NO after the decomposition of N_2O in the H_2 - N_2O reaction were measured by UV absorption behind incident normal shock waves in a 6-inch ID stainless steel shock tube. They observed that the OH profiles had qualitatively similar features to those in the H_2 - O_2 reaction. They stated that the chain reaction in the H_2 - N_2O reaction was initiated by the O atoms generated by the unimolecular decomposition of N_2O , reaction R2, which then reacted with hydrogen as in reaction R4. A key finding from this study was that the calculated NO concentrations were much smaller than those observed experimentally and this difference increased with a decrease in temperature and an increase in the $[H_2]/[N_2O]$ ratio. This identified the major defect in the reaction mechanism to be the incorrect description of NO formation. Their experiments also supported the fact that the NO concentration remains constant after the consumption of N₂O. In addition to this, an earlier study on the decomposition of N₂O [37] did not detect NO₂, thereby supporting the insignificance of reaction R5.

$$N_2O + M \longrightarrow N_2 + O + M$$
 (R2)

$$N_2O + H \longrightarrow N_2 + OH$$
 (R3)

$$O + H_2 \longrightarrow OH + H$$
 (R4)

$$NO + N_2O \longrightarrow NO_2 + N_2.$$
 (R5)

Thus, Henrici and Bauer concluded that NO is produced in reaction R13 and is not involved in any further reactions. The rate constant they determined for the NO formation reaction R13 was larger than previously determined values from studies on N₂O decomposition, N₂O-fuel reactions and N₂O-O reactions.

Further investigation by Soloukhin in 1973 [38] on the oxidation of hydrogen by nitrous oxide in shock waves at temperatures of 1400-2300 K showed the importance of OH^{*} in the chemical kinetics of H₂-N₂O mixtures. The recorded absolute rates of rise and decay in the OH^{*}-emissions were higher than those obtained in numerical calculations for OH. They were also compared to the measurements of OH-concentration profiles from the prior study by Henrici and Bauer [36] as the differences they observed between calculated and experimental values of OH were less significant. This led to a reasonable assumption that the profiles of $OH^*(^{2}\Sigma)$ and OH do not coincide, and that the collisional quenching times for OH^{*} are shorter than the overall reaction times. Based on this argument, the author concluded that the high rates of OH^{*} formation, through reaction R6, must be taken into account in evaluating the overall rates of radical generation in a reaction mechanism.

$$H + N_2 O \longrightarrow OH^* + N_2$$
 (R6)

This reaction explained the high rates of OH^* production observed in an earlier study by Soloukhin and Van Tiggelen [39]. Thus, Soloukhin concluded that R6 is a key chain branching path for the hydrogen-nitrous oxide system based on their shock tube measurements. The role of OH^* radicals in this mixture was also previously postulated by Duval and Van Tiggelen [40] when studying H₂-N₂O flames.

Decades later, in 2015, Mével and Shepherd [41] investigated the ignition delays of small hydrocarbon-N₂O mixtures with and without O₂ using shock-tube experiments. The chemical kinetic simulations presented in this work included an OH^{*} sub-mechanism. They argued that the concentration of OH^{*} is typically 6 orders of magnitude lower than that of OH radicals, and so the inclusion of OH^{*} chemical pathways would not significantly modify the ground-state chemistry. Additionally, a number of past studies [13, 38–40, 42–45] had demonstrated that the chemical pathways forming OH^{*} radicals differ from those forming the ground-state OH radical, and so it was important to include a sub-mechanism for their chemistry when modeling ignition delay-times based on OH^{*} emission.

In mixtures with only N_2O as the oxidizer, Mével and Shepherd [41] concluded that the two dominant reactions are R2 (promotes the overall reaction through the production of reactive O atoms [26]) and R3. The other important reactions all involved consumption or production of the H atom. In these mixtures, OH radicals were formed almost exclusively by R3 and the ignition was due to a thermally driven linear chain process which involved R2 and R3 [42]. With respect to OH^{*} in mixtures

$$CH + O_2 \longrightarrow CO + OH^*.$$
 (R7)

In both cases (N₂O and N₂O+O₂ as oxidizer), the energy release was dominated by the very exothermic reaction R3 [41], as shown in Figure 2.3. In the case of mixtures which contained only N₂O, the thermal decomposition of nitrous oxide played a significant role in absorbing heat. The reaction rate of this process increased as the overall reaction proceeded because of the mixture temperature increase. In the case of mixtures which contained both N₂O and O₂, the nitrous oxide decomposition was not significant in the energy release. In these mixtures with both N₂O and O₂, in addition to R3, three other reactions contributed to the temperature increase:

$$OH + H_2 \longrightarrow H_2O + H,$$
 (R8)

$$CO + OH \longrightarrow CO_2 + H,$$
 (R9)

$$C_2H_2 + O \longrightarrow T - CH_2 + CO$$
 (R10)

$$H + O_2 \Longrightarrow OH + O.$$
 (R11)

As the reaction accelerates and increasing amounts of OH radicals are produced, the contribution of the endothermic branching involving H and O_2 , reaction R11, in absorbing heat increases. Finally, sensitivity and reaction pathway analyses demonstrated that ignition is mostly driven by R2 and R3, for mixtures with only N₂O, and by R3 and R11 for mixtures which include oxygen as well. The good agreement between experimental and calculated values obtained by Mével and Shepherd motivated the use of their reaction mechanism for calculating theoretical parameters in the current work.



Figure 2.3. Energy release per reaction analysis for experiments with single-peak emission profiles [41]. (a) CH₄-N₂O, $\phi = 1.11$; (b) C₂H₆-N₂O-O₂, $\phi = 1.12$.

Few researchers also studied the chemical kinetics of hydrocarbon-nitrous oxide systems. To investigate the chemical pathways for reaction of hydrocarbon species with N₂O, Vandooren et al. [25] compared and discussed them using argon-diluted methane flames with O₂ and N₂O as oxidizers. Their observations showed that the maximum concentrations of CH₃, CH₂O and C₂H₂ were similar in both flames indicating similar pathways in the carbon chemistry with O₂ and N₂O. A difference they observed was in the behavior of oxygen and hydrogen species in the two flames. Molecular oxygen (O₂) was formed in the CH₄-N₂O-Ar flame, but was only consumed in the CH₄-O₂-Ar flame. They also measured lower concentrations of O and H and higher concentration of OH in the N₂O flame which they attributed to the nearly irreversible reactions R12, R13 and R3. This was in contrast with the reversible reaction R11 which occurs in the O₂ flame.

$$N_2O + O \longrightarrow N_2 + O_2$$
 (R12)

$$N_2O + O \longrightarrow NO + NO$$
 (R13)

In the same year, Zabarnick [46] compared $CH_4/NO/O_2$ and CH_4/N_2O flames by LIF diagnostics and confirmed the conclusions made by [25]. They highlighted the importance of reactions R2 and R3 as key pathways for the consumption of N₂O and production of OH. As discussed in Section 2.2.1, Powell et al. [30] studied the chemical kinetics of hydrogen and small chain hydrocarbons with nitrous oxide where they highlighted the importance of N₂H_x/NH_x reactions in the overall mechanism. The main reactions from the CH_4/N_2O system from [30] are shown in Table 2.1 to compare with the CH_4/O_2 system.

Chemical kinetics studies on systems using nitrous oxide as the oxidizer have revealed that the decomposition reactions, R2 and R3, are important as initiation and exothermic pathways, respectively. Some works have established that the inclusion of OH* in the nitrous oxide mechanism provided better agreement between calculations and experiments. In comparison, the reaction with oxygen follows a chain branching process whereas with nitrous oxide there is a linear chain process whether the fuel is hydrogen or methane, as shown in Table 2.1, and this can be extended to most small chain hydrocarbons, at least. In addition, the initial exothermic behavior in mixtures with oxygen as the oxidizer is due to reaction R11, but in nitrous oxide systems it is due to reaction R3. In systems with hydrocarbons as the fuel, the initiation process also includes H abstraction from the fuel molecule and the H atoms then participate in chain branching reactions. Overall, the carbon chemistry follows similar pathways in both oxygen and nitrous oxide reactions with small chain hydrocarbons.

2.2.3 Nitrous Oxide Decomposition

The exothermic decomposition of nitrous oxide is a unique feature of this oxidizer and is triggered at temperatures higher than approximately 830 K. This behavior of nitrous oxide is particularly relevant to the current study because it can potentially decompose due to heating caused by the pre-compression of the unburned gas mixture

H_2-O_2	H_2-N_2O [14]	
$H_2 + O_2 \longrightarrow 2OH$	$N_2O + M \longrightarrow N_2 + O + M$	
$H_2 + O_2 \longrightarrow HO_2 + H$	$O + H_2 \longrightarrow H + OH$	
$OH + H_2 \longrightarrow H_2O + H$	$N_2O + H \longrightarrow N_2 + OH^*$	
$H + O_2 \longrightarrow OH + O$	$N_2O + H \longrightarrow N_2 + OH$	
$O + H_2 \longrightarrow OH + H$	$OH + H_2 \longrightarrow H_2O + H$	
CH_4-O_2 [47]	CH_4 - N_2O [30]	
$CH_4 + H \longrightarrow CH_3 + H_2$	$CH_4 + H \longrightarrow CH_3 + H_2$	
$CH_4 + OH \longrightarrow CH_3 + H_2O$	$CH_4 + OH \longrightarrow CH_3 + H_2O$	
$CH_4 + O_2 \longrightarrow CH_3 + HO_2$	$N_2O + M \longrightarrow N_2 + O + M$	
$H + O_2 \longrightarrow OH + O$	$N_2O + H \longrightarrow N_2 + OH^*$	
$O + H_2 \longrightarrow OH + H$	$N_2O + H \longrightarrow N_2 + OH$	
$ O_2 + CH_3 \longrightarrow CH_2O + OH$	$N_2O + O \longrightarrow N_2 + O_2$	

Table 2.1. Comparison of important reactions between hydrogenoxygen and hydrogen-nitrous oxide systems and methane-oxygen and methane-nitrous oxide systems.

ahead of the accelerating flame or due to hot spots formed in the unburned gas mixture.

The decomposition characteristics of nitrous oxide have been studied by many researchers, primarily to isolate significant reactions and to improve their rate constants over varying initial conditions. Hidaka et al. [48] measured species concentrations in shock-tube studies of N₂O decomposition and N₂O-H₂ reaction, and derived improved rate constants for some of the elementary reactions in the temperature range of 1450-2200 K. They verified the rate expression for the unimolecular N₂O decomposition reaction, R2, with rates available in the literature at that time and derived improved rate constants for three important reactions, R12, R13 and R3, involving N₂O. A main conclusion of their work was that the decomposition of N₂O is insensitive to the rate constants of R12 and R13 as N₂O consumption was primarily through R2. In contrast, they observed that the product concentrations of the N₂O-H₂ system were sensitive to the rate constants of these two reactions. These conclusions stressed the importance of reaction R2 as the initiation step in systems using N₂O. Another important study on nitrous oxide decomposition was conducted by Allen et al. [49] and was significant due to their investigation into the pressure dependence of this process. They varied the flow reactor pressure over a range of 1.5-10.5 atm with temperature varying in the range 1103-1173 K and measured different species profiles. The authors then conducted reaction flux and sensitivity analyses to determine the rate controlling steps, thereby modifying reaction rate constants to match experimental values. Their analysis showed that N₂O was consumed entirely through two pathways: (1) unimolecular decomposition of N₂O (R2) and (2) its reactions with O atoms (R12 and R13). However, the unimolecular decomposition of N₂O controlled the overall rate of consumption and the measured N₂O depletion profiles at 1123 K showed that the N₂O decomposition rate increased with pressure. They explained the high rate of N₂O depletion through the following chemical pathway: at reaction initiation, nearly 100% of N₂O is consumed through the unimolecular decomposition reaction. Once O atom concentration increases, the reactions involving N₂O and O atoms (R12 and R13) become significant. Later, as NO accumulates, the reaction

$$NO + O + M \longrightarrow NO_2 + M$$
 (R14)

competes strongly with reactions R12 and R13 for O atoms. The study showed that at 90% reaction completion point, the unimolecular decomposition reaction was responsible for the high rate of N_2O consumption. Based on the measured species profiles, the authors improved the rate constant expression for this decomposition reaction at high pressures by increasing it by a factor of 3 from values available in the literature.

Around the same time, Röhrig et al. [50] conducted another study on the pressure dependence of thermal decomposition of N₂O for a temperature range of 1570-3100 K and a pressure range of 0.3 - 450 atm. Their results showed that the pressure dependence of N₂O consumption above 6 atm was not linear and that the rate coefficients in this region are in the fall-off range. They extrapolated the rate constant for reaction R2 from Allen et al. [49] to their temperature range and observed a moderate agreement with their experimental fall-off curves up to a pressure of 50 atm only, with deviations at higher pressures. They attributed this deviation to real gas effects for experiments at pressures above 100 atm, which Allen and coworkers did not consider. Also, at temperatures above 1700 K, Röhrig et al. [50] observed an increase in the reaction rate of R2 in relation to the sum total of the rates of R12 and R13 due to the higher activation energy of R2.

In addition, Javoy et al. [51] studied the N_2O decomposition rate constant at high temperatures and showed that at temperatures above 2500 K, the decomposition rate is too fast to be accurately evaluated. They also ranked the roles of reactions R12 and R13 in the low- and high-temperature ranges and stated that reaction R12 was dominant at temperatures below 1850 K and R13 was significant at temperatures above 1850 K. This difference in reaction dominance between reactions R12 and R13 was explained using equilibrium composition calculations.

A discussion on the decomposition behavior of nitrous oxide in a combustible mixture was provided by Mével et al. [33] who conducted chemical kinetics modeling on H₂-N₂O-Ar mixtures. They noted an important difference in the reaction pathway of N₂O during auto-ignition versus flame propagation - the thermal decomposition of N₂O was only important for the auto-ignition process and not for flame propagation which they attributed to diffusion of H atoms ahead of the flame front. For autoignition, N₂O first decomposes to produce O atoms which then react with H₂ to break the strong H-H bond. The H atoms then react with nitrous oxide through reaction R3 producing OH which reacts with hydrogen molecules to further produce H atoms, leading to a fast energy release through a linear chain pathway. However, in propagating flames, H atoms diffuse ahead of the flame front and react with nitrous oxide mainly through reaction R3 allowing the energy to be released. Thus, the pathways R2 and R4 are almost suppressed because of diffusion of the H atoms in propagating flames. All these studies on the decomposition of N_2O have effectively concluded that reactions R2, R12 and R13 are the most important elementary steps involved in the decomposition process and have provided improved rate constants for these reactions. The overall rate of decomposition of N_2O increases with increase in pressure and temperature. These works also highlight the role of each of these reactions as a function of temperature of the decomposition process.

2.3 Application of Nitrous Oxide Detonations

Based on the reviewed applications of detonations in nitrous oxide, measurements from this work affect three broad fields of study: safe handling of nitrous oxide, geothermal stimulation and rocket propulsion.

One of the aims of this work was to add to the existing database of knowledge on nitrous oxide detonations with a focus of mitigating explosions in the nuclear waste management industry and in gas delivery systems. The work done at the Explosion Dynamics Laboratory at Caltech [10–12] made immense progress in this area. Their motivation was the presence of flammable gases in nuclear waste storage tanks at Hanford, WA, one of which is nitrous oxide. The experiments they conducted provide a reliable database of detonation properties with nitrous oxide as the oxidizer at sub-atmospheric initial pressures.

As an extension of this work, stoichiometric ethylene-nitrous oxide was earlier tested as a geothermal stimulant to fracture rock [52,53]. This work involved the development of a two-component energetic gas mixture that can be injected down-hole to enhance well bore permeability. This technique demonstrated a method of injecting a tailored mass of ethylene-nitrous oxide mixture into the well bore and successfully initiating combustion in the mixture. Prompt transition from deflagration to detonation was observed within a pressure range that would induce fractures in the well bore wall without causing formation damage (rubble, well bore collapse). Detonation of the mixture within the well bore significantly increased the measured well bore volume as a result of the numerous fractures generated. The detonation pressures measured in the well bore were higher than the CJ values due to pre-compression of the unburned gas mixture prior to deflagration-to-detonation transition (DDT) [54, 55]. Each subsequent "stimulation shot" increased well bore volume through additional fracture volume, the largest increase corresponding to higher initial pressures and higher detonation pressures as would be expected.

A simple back "mining" operation conducted to map the location of the fractures surrounding the well bore confirmed that this technique effectively generates a high surface area network of fractures. These fractures were formed by a high-energy combustible gas mixture which caused shear displacement and erosion in the rock. Due to this, the fractures were self-propping. Comparing this stimulation method to hydraulic fracturing and deeply buried solid explosive fracturing methods, this method produced peak pressures comparable to those seen in hydraulic fracturing, but significantly lower than those produced by solid explosives. Additionally, these gaseous detonations propagated and produced consistent loading down the wellbore as opposed to a concentrated, high impact loading from solid explosive fracturing leading to the possibility of mechanical damage of the casing and well [56].

In terms of propulsion, the usage of nitrous oxide dates back to the 1930s when a nitrous oxide and coal hybrid rocket was developed and tested at I.G. Farben in Germany. It produced 10 kN thrust for 120 s [57]. This was followed by its usage in Luftwaffe aircraft engines during World War II to improve high-altitude performance. The gas was chilled, liquefied and sprayed under pressure into the engine intake manifold using the system known as Göring Mischung 1 or GM-1. Around the same time, NACA investigated supercharging radial engines with nitrous oxide [58].

Following the work done by Laughrey et al. [7], in 1963, Jost et al. [59] studied the detonation and chemical kinetics of hydrazine and nitrous oxide to assess the viability of nitrous oxide as an oxidizer for rocket propulsion. They measured detonation speeds of hydrazine-nitrous oxide mixtures at low initial pressures on the order of 0.1 atm and found the speeds to be near the ideal Chapman-Jouguet (CJ) detonation

velocity, but observed that these detonations were unstable. Additional interest in nitrous oxide had arisen in the past several years as an oxidizer for rocket propulsion systems. However, accounts of serious, large system nitrous oxide accidents described in [60, 61] highlight the hazards associated with nitrous oxide and the oxidizer must be handled with utmost care free from impurities, as with any good oxidizer. As described in the Airgas investigative report [61], since the decomposition of nitrous oxide is exothermic, this process is self-sustained and can lead to explosions. This warrants intimate understanding of the oxidizer and its combustion properties with different fuels prior to using it as a propellant.

In the late 1980s, Grubelich et al. [62] replaced toxic or cryogenic oxidizers typically used in hybrid engines with nitrous oxide and tested it with hydroxyl terminated polybutadiene (HTPB) as the fuel. According to their work, the nitrous oxide hybrid engine can have longer burn times than conventional solid propellant rocket motors for a given geometry. Several years later in 2001, Tyll et al. [63] tested nitrous oxide with propane in a bipropellant rocket engine. The nitrous oxide was catalytically decomposed and this exothermic process ignited the propane to produce sustained combustion. Tyll and co-workers proposed that performance improvements could be achieved by replacing the low vapor pressure propane with ethylene, which had a similar vapor pressure as nitrous oxide. Using ethylene as the fuel, their analysis predicted an increase of the specific impulse by several seconds. In addition, DiSalvo et al. [64] tested their patented constant volume rocket motor with nitrous oxide and propane in pulsed motor mode generating brief chamber pressure pulses on the order of 500-700 psia using injector inlet pressures of only 40-50 psia. In 2011, DARPA announced the Airborne Launch Assist Space Access (ALASA) program designed to produce a rocket capable of launching a 100 lb. satellite into low earth orbit with Boeing contracted to develop the launch system. Boeing intended to lower the complexity of the launch vehicle and thus costs by powering the rocket with a monopropellant comprised of a pre-mixed combination of nitrous oxide and acetylene [65]. As of 2015, DARPA terminated this program due to explosions of the pre-mixed propellant during ground tests. Both nitrous oxide and acetylene are very energetic and individually function as mono-propellants. This intensified the complexity associated with storing a premix of these gases. The author of this thesis **does not** recommend storing nitrous oxide as a pre-mixed combination with any fuel due to the highly unstable explosions resulting from nitrous oxide mixtures. However, the objective of the ALASA project provides another example of nitrous oxide's popularity as an oxidizer.

Werling et al. [66] at the German Aerospace Center (DLR) recently developed an ethylene-nitrous oxide premixed rocket engine as a replacement for today's hydrazine engines. Their choice of ethylene as fuel was driven by the similar vapor pressures of ethylene and nitrous oxide, which was also suggested by [63]. This similarity in vapor pressures assured good miscibility and simultaneous evaporation of the propellants in the tank. They tested this mixture at oxidizer-to-fuel (O/F) ratios in the range of 8.5 to 11, with stoichiometric ratio being 9.42. In their tests, they achieved a C^* efficiency of 92% with an average measured C^* of 1480 m/s.

To summarize, investigations of detonations involving nitrous oxide have been limited to using it as a monopropellant or in a bipropellant mixture with hydrogen [13, 14, 67]. Additionally, there have been some studies on the decomposition of pure nitrous oxide either due to homogeneous heating of the gas or from local thermal ignition [68, 69], and these have been studied using chemical mechanisms discussed previously in this chapter. These studies help predict and explain combustion trends in nitrous oxide-fuel mixtures better, and provide some information on flammability limits. Available literature on nitrous oxide-hydrocarbon detonations is mainly restricted to initial pressures below one atm. or with dilution [70]. Therefore, detonations with nitrous oxide as the oxidizer are far from being completely characterized. In addition to this lack of general knowledge, understanding of nitrous oxide-fuel detonations at higher pressures, more typical of practical combustion systems is either extremely limited or non-existent. Several of the studies discussed earlier suggest benefits of using nitrous oxide in a bipropellant mixture with small hydrocarbons such as propane, ethylene and acetylene for propulsion systems, but no information is available on the detonation properties of these mixtures. Records of measured detonation properties of these fuels with O_2 -diluents [16, 21, 71–76] and air [15, 77–79] are available and provide an order of magnitude estimation of their properties with nitrous oxide. Hence, in order to apply these fuel-nitrous oxide mixtures to practical detonation systems, their detonation properties have to be studied over a wide range of initial conditions, which include pressure, temperature, ignition energy and dilution.

In particular, fuel-N₂O detonations can be used in a gas-phase blow-down thruster. In such a system, compressed fuel and oxidizer are stored separately and are individually fed into the chamber in gas phase. Finally, the chamber is isolated from the propellant tanks before igniting and the hot gases are allowed to blow down through a nozzle. The closed combustion tube used in this study replicates such a system. If this process is cycled, the system works as a pulse detonation engine. As a first step towards addressing this knowledge gap, the current work focuses on the characterization of detonations in undiluted ethylene-N₂O as a function of initial pressure in a closed combustion tube. This will add to the existing database of knowledge on nitrous oxide detonations, thereby enabling the robust design of gas delivery and propulsion systems that can operate with N₂O. The measurements from this work are compared to the theoretical Chapman-Jouguet detonation parameters, and deviations of the experimental results from the theoretical predictions are discussed. Additionally, the results are compared to the performances of ethylene-O₂ mixtures as a baseline.

3. METHODS

An experimental investigation of detonations requires a robust combustion chamber to contain the high pressures and temperatures associated with such phenomena. For this purpose, two such experimental test rigs are designed and fabricated in-house. One is a completely closed, circular cross-section tube with no visualization windows, but capable of studying detonations with initial pressures higher than 1 atm. This test rig is located at the High Pressure Laboratory at Maurice J. Zucrow Laboratories. For convenience, this tube is designated C1. The other test setup, designated C2, is a rectangular cross-section tube with full-length windows to study flame acceleration in mixtures at initial pressures around 1 atm. This experiment is located at the Aerospace Sciences Laboratory. This chapter describes the design of the combustion tubes, the propellant delivery system, the ignition methods used, the instrumentation used to study the detonations and the procedure followed to run these experiments.

The current design of combustion tube C1 is motivated by similar tests conducted in a smaller L/d (= 6.13) combustion tube, designated C0. The data from these earlier tests in the small L/d combustion tube indicate inconsistent pressures between tests of the same initial pressure. In addition to this, overdriven detonations are observed and the short tube does not allow the detonation to decay to a stable state. The pressure recorded from these earlier tests will be discussed briefly in Chapter 5. Thus, in order to observe and study steady detonations, a combustion tube with a larger L/d of 68 is designed and fabricated. This combustion tube is used to investigate the consistency in detonation parameters between tests of same initial pressures for a stoichiometric mixture of ethylene and nitrous oxide.

3.1 Combustion Tube C1

3.1.1 Tube Design

The combustion tube used for these experiments is 75 inches long with an inner diameter of 1.1 inches (L/d = 68) and is closed at both ends. It consists of three separate sections integrated together using two full-depth welds. The central tube section is fabricated using a 75 inch long, 1.5 inch XX-Heavy pipe. This pipe has an inner diameter of 1.1 inches and is rated to a working pressure of 7,200 psi and a burst pressure of 25,300 psi. To accommodate 12 high-frequency pressure transducers, $3/16^{th}$ inch holes are drilled, 6 inches apart, along the length of the tube. These details are shown in the engineering drawing in Figure D.1 in Appendix D.

The other two sections of the combustion tube are fabricated using stainless steel 304 blocks and have 3 inch by 3 inch cross sections and are 3.5 inches long. These sections each contain three F375C ports used to attach propellant and nitrogen delivery plumbing, thermocouples and exhaust plumbing. In one of these block sections, a port to accommodate another high-frequency pressure transducer is machined axially at the dead end. The other block section includes a port to install the igniter adapter used to accommodate different ignition methods and an optic port. Engineering drawings of these two block sections are given in Figures D.2 and D.3 in Appendix D.

As mentioned earlier, the three sections are integrated together using full-depth welds to ensure strength. In addition to the three main sections, the construction of the combustion tube consists of 12 pressure transducer adapters to install PCB[®] 109C11 high-pressure transducers. These are similar in dimensions to the pressure transducer port on the propellant delivery block section and are detailed in Figure D.4. These adapters are welded onto the central tube section concentric with the $3/16^{th}$ inch holes drilled along the length of the section. A schematic of this assembly is shown in Figure 3.1 and the actual combustion tube assembly is shown in Figure 3.2. The assembled combustion tube is hydrostatically tested to 10,000 psi without any damage to the welds. The combustion tube is then installed onto the test stand and held in place using two vibration-damping brackets.



Figure 3.1. Diagram of the assembled combustion tube with basic dimensions.



Figure 3.2. Welded combustion tube prior to assembly on the test rig.

3.1.2 Gas Delivery System

The gas filling system consists of three separate plumbing lines for fuel, oxidizer and nitrogen. The high pressure nitrogen supply from the lab, regulated to 300 psi, is used for purging combustion products from the tube after each test and a separate 100 psi nitrogen line is used as pilot pressure for all the pneumatic valves on the test stand. Ethylene and nitrous oxide (or oxygen) are supplied from their respective bottles via the other two plumbing lines. The propellant bottles are installed with manual regulators in combination with inlet and outlet pressure gauges to set the desired



Figure 3.3. Experimental test rig with combustion tube and propellant delivery panel.

propellant supply pressure. Each propellant line is equipped with a pneumatic ball valve, a relief valve and a check valve before it is connected to the combustion tube. In addition to these flow devices, low-frequency pressure transducers, thermocouples and sonic venturis are installed on the propellant lines to set the mass flow rate of the propellants.

The relief values ensure that the pressure in each line is well below the pressure rating of the flow device with the lowest value, thereby preventing any damage or rupture of the lines. The check values are connected at each gas inlet on the propellant delivery end block of the combustion tube to prevent back flow of unreacted mixture and combustion gases into the supply cylinders. The low-frequency pressure transducers and thermocouples are used to maintain and monitor the pressures upstream of the sonic venturis, which allow fixed mass flow rates of the propellants resulting in the appropriate final pressure and equivalence ratio for each test. The fuel and oxidizer gases flow into the tube from opposing ports to facilitate mixing of the gases. The valves and sonic venturis are mounted on an aluminum panel as shown in Figure 3.3.

The vent line is attached to the vent port on the ignition end of the combustion tube. This line consists of a rupture disc assembly, a high-pressure pneumatic ball valve to contain the combustion gases and another pneumatic ball valve to contain the combustible mixture prior to ignition. A low-frequency static pressure transducer is installed in between these two pneumatic ball valves and is used to monitor and measure the pressure in the combustion tube during the propellant fill process. All components of the plumbing and propellant delivery systems are shown in a schematic plumbing and instrumentation diagram (P&ID) in Figure 3.4. A summary of the feed system instrumentation is given in Table 3.1 with each component's respective designator on the P&ID as shown in Figure 3.4. These instruments are all connected to the low-speed data system which records data at 100 Hz.

Table 3.1. Summary table of low-speed instrumentation on the experimental setup as indicated by designator in P&ID

Designator	Description	Туро	Bango
Designator	Description	туре	Italige
PT-FU-901	Fuel Pressure Upstream of Sonic Venturi	Druck PMP-1260	0-3000 psia
PT-OX-901	Oxidizer Pressure Upstream of Sonic Venturi	Druck PMP-1260	0-3000 psia
PT-N2-901	Pre-fire Combustion Tube Pressure	Druck PMP-1260	0-500 psia
TC-FU-901	Fuel Temperature Upstream of Venturi	Omega K-Type	$0-160^{\circ}\mathrm{C}$
TC-OX-901	Oxidizer Temperature Upstream of Venturi	Omega K-Type	$0-160^{\circ}\mathrm{C}$
TC-CT-901	Combustion Tube Temperature at Igniter End	Omega K-Type	$0-160^{\circ}\mathrm{C}$
TC-CT-902	Combustion Tube Temperature at Dead End	Omega K-Type	$0-160^{\circ}\mathrm{C}$

3.1.3 Ignition Methods

One objective of this work is to investigate the ignition of ethylene-nitrous oxide mixtures with a low-energy ignition source and compare it to ethylene-oxygen mixtures. Two different ignition methods are explored. The first method is a modification of the low-energy ignition source utilized in the tests conducted in the small L/d combustion tube. The bi-propellant mixture in these preliminary tests was ignited by heating a 3.5-inch long nichrome wire [6] or an e-match. The bi-propellant mixture in tube C1 is ignited by heating a nichrome wire 1/8 in. long soldered to the leads of a Kemlon[©] feed-through fastened into the igniter adapter in the tube front end wall. The feed-through with the nichrome wire is shown in Figure 3.5(a). The nichrome wire is heated using an 18 VDC Li-Po battery switched on by a solid state relay. Once the wire reaches a critical temperature it breaks away from one of the leads, indicated by the white region in the schlieren image in Figure 3.5(b), and results in the fragmentation of the hot wire. The heat generated by the wire thermally ignites the gas mixture and initiates a deflagration.

The second method to ignite the bi-propellant mixture is with an automotive spark plug using a high voltage spark ignition circuit fabricated in-house [80]. The circuit diagram for this is shown in Figure 3.6. The circuit has the capability to produce high-energy (up to 0.5 J) pulses at voltages up to 45 kV. This allows for spark discharge under the high initial pressures used in this work. The circuit is an integration of three sub-circuits: a voltage conditioning circuit, capacitor charging circuit, and discharge triggering circuit. The voltage conditioning circuit transforms the 120 VAC supply voltage to 300 VDC for use in the charging and triggering circuit. The capacitor charging circuit consists of a relay which closes with a remote, 5 VDC "Arm" signal to charge a capacitor to 300 VDC, storing a specified amount of electrical energy. The discharge triggering, or "firing" circuit, uses an external TTL signal to trigger the capacitor to discharge through a high voltage pulse transformer, which initiates electrical breakdown across the electrode gap [80]. The spark discharge circuit is connected to a standard Denso[©] IW20 spark plug with an iridium electrode shown in Figures 3.7(a) and 3.7(b). Different igniter adapters are fabricated for each ignition method in use and the adapters have an extra port to introduce an optic fiber as shown in Figures 3.7(a) and 3.7(b).

3.1.4 High-Frequency Instrumentation

The combustion tube C1 can accommodate 12 high-frequency PCB[®] 109C11 pressure transducers in ports on the sidewall. The first pressure transducer port is 4.378 inches from the igniter plane and the rest are evenly spaced 6 inches apart down the tube length, to measure pressure peaks during the propagation of the combustion wave. Out of these 12 ports, 10 have pressure transducers installed in them. The remaining two ports, farther from the ignition location, are plugged as the propagating combustion wave is stable in this region and fewer data locations are sufficient to measure detonation properties. One pressure transducer is installed in the end wall to measure the reflected pressure. These transducers have a measurement range of 0-80,000 psi with a useful over-range of 0-100,000 psi and are connected to the highfrequency data acquisition system at the High Pressure Lab of Maurice J. Zucrow Labs to record pressure at 600 kHz/channel. The manufacturer of these senors specifies a non-linearity of $\leq 2\%$ full scale output and a resolution of ≤ 2 psi.

The PCB[®] pressure transducers are dynamic sensors and are well suited to measure steep fronted pressure waves. This prevents them from accurately measuring the pressure rise from the compression waves produced by the accelerating flame. In order to measure this pressure rise, two quasi-steady state pressure transducers from Kulite[®] are installed in plane with the first two PCB[®] transducers (closest to the ignition plane) and at 90° from them. The two Kulites used in these locations are the CT-375 and XTEL-375 models which have a range of 3000 and 2000 psi, respectively. These models are chosen purely based on availability of senors with the required pressure range in the lab. Kulite[®] specifies a non-linearity of $\pm 0.1\%$ full scale output and an infinitesimal resolution for both models. The Kulite[®] pressure transducers are also sampled at 600 kHz on the lab high-frequency data acquisition system.

Another sensor used in this study is a photo-multiplier tube (PMT) module. A propagating flame emits light and this can be detected using either a photodiode or a PMT module. For this study, a PMT module (Hamamatsu[©] part # H11903-210) is

used to record light emitted by the propagating flame. A local explosion arises within the shock-flame complex when this propagating flame transitions to a detonation, and this phenomenon was first observed and visualized by Urtiew and Oppenheim [81]. During this deflagration-to-detonation transition (DDT), the explosion emits a sudden burst of light, which the PMT module captures, and this inflection in the light intensity signal defines the time of onset of detonation. This inflection time is synchronized with the high-frequency pressure measurements to estimate the run-up distance. This method of detecting the onset of DDT was used in prior studies on experimentally measuring DDT [17–20], but using a photodiode for light detection instead of a PMT module. To implement this method for the current work, the light from the combustion tube is captured using a fiber optic installed in the igniter adapter. The light is them passed through narrowband and neutral density filters to efficiently analyze the signal without noise. The signal from the PMT module is recorded using the high-frequency data acquisition system at 600 kHz.

The optical port configuration is shown in Figure 3.8. The design of the optic port in the igniter adapter is derived from the work of Bedard [82] and the following description is adapted from his thesis with permission. A $1/16^{th}$ inch aperture allows light to propagate through the adapter wall and through a $1/8^{th}$ inch thick sapphire window which is cushioned against the bottom of the port by a 0.015 inch thick brass washer. The sapphire window provides protection for the fiber optic while allowing ultraviolet wavelengths to pass. The window is secured in the port using a threaded brass retainer. The retainer is machined to provide uniform compression of the window. A counter bore at the top of the retainer holds the tip of the fiber optic probe such that it is aligned with the centerline of the optic port. A 0.030 inch aperture is drilled through the center of the retainer to provide the limiting aperture to the optical fiber's field of view. Two igniter adapters with an optic port and the respective igniter port are machined for this work and their cross-sectional views are shown in Figure 3.9. The optical fiber is a 400 μ m core fused silica fiber that is mounted in a 1/8th inch diameter stainless steel ferrule. The steel ferrule provides protection for the fiber and enables the optical port pressure seal to be formed on the outer wall of the igniter adapter using a compression fitting as shown in Figure 3.8. The 12 ft. length of the optical fiber is jacketed with PVC to provide a durable and bend resistant covering. The other end of the fiber is terminated with a standard SMA connector for connection to the filtering optics. Light entering the optics assembly from the fiber first enters a collimating lens (Thorlabs[©] part # LB4280-UV) to reduce the divergence angle of light emitted from the fiber before reaching the PMT module. In addition to the setup in [82], a neutral density filter is added downstream of the collimating lens which reduces the light intensity by 90%. The light from the combustion and eventual detonation is intense enough that it saturates the PMT sensor which prevents the detection of DDT. So, the filter ensures sufficient light to fall on the sensor to detect the flame to detonation transition.

3.1.5 Test Procedures

The tube and the propellant lines are heated to 100°F using tape heaters to prevent condensation of the propellant gases at high pressures. Since the experimental setup is outdoors where the ambient temperature fluctuates over a year, these tape heaters also ensure that the propellants in the delivery lines and in the combustion tube are maintained at the same temperature for all tests conducted in this study. The propellant fill procedure begins with a purge of the tube with the oxidizer (nitrous oxide or oxygen). The vent valve is closed and the tube is pressurized to 30 psia with the oxidizer. At this point, a fixed venturi vacuum ejector (VACCON[©] Min J Series) using 100 psia nitrogen on its vent line evacuates the combustion tube to a pressure of about 2 psia. This process ensures that the tube is devoid of air or residual combustion products prior to propellant fill and the approximately 2 psia remaining in the tube is oxidizer. After purging and evacuating, fuel and oxidizer are flowed simultaneously from opposite ports to achieve a stoichiometric fuel-oxidizer mixture at the desired initial pressure. The flow rates of the propellants are controlled by the pressures upstream of the sonic venturis in each delivery line and the propellants are flowed for the same amount of time. The flow period is determined based on the target initial pressure, mixture ratio and the allowable upstream pressures to ensure choking of the sonic venturis. After pressurizing the tube, a dwell period of 45 s is maintained to allow any condensed gases to evaporate and allow for diffusion mixing of the propellants.

Figure 3.10 shows fuel, oxidizer and combustion tube pressures during a typical test. At the end of the dwell period, the LabVIEW VI used to remotely control the experiment actuates the ignition circuit to either energize the nichrome wire or initiate discharge across the electrodes of the spark plug, depending on the ignition method. This ignites the combustible mixture, producing a deflagration wave which propagates down the tube, transitioning to a detonation when the flame reaches the appropriate DDT criteria for the mixture. At the end of each test, the high-pressure vent valve is opened and nitrogen is flowed through the tube for 2-3 minutes to purge the combustion gases and prepare the tube for the next test. The recorded signals from high-frequency pressure transducers and the PMT module are then processed using a data reduction code in MATLAB[®] for analysis. This procedure is followed consistently for all tests to maintain uniformity and minimize uncertainty due to operations.

3.2 Combustion Tube C2

Combustion tube C1 is designed to study detonations in mixtures with initial pressures several times higher than atmospheric pressure. Due to this criteria, optical accessibility to study different features of flame acceleration is a challenge. So, to investigate this phenomenon a second combustion tube, C2, is designed and fabricated in-house.

3.2.1 Tube Design

The combustion tube used for this phase of the project is designed with the following criteria: full-length optical accessibility, planar windows to allow schlieren imaging of the flow-field and sufficiently long to observe ignition, flame acceleration and DDT. Based on these criteria, this tube has a rectangular inner cross-section of height 1.01 inches and width 0.74 inches, and is 29.5 inches in length. The design includes several different parts which are fastened together to form the combustion tube and so provides a level of modularity if the dimensions need to change for different mixtures.

Two $3/8^{th}$ -inch thick polycarbonate sheets are fastened onto two aluminum-6061 square cross-section bars of 0.74×0.74 inch, which forms the inner width. The aluminum bars are separated by 1.01 inches to form the height. O-ring cord stock of 0.103-inch thickness is used to create a seal between the polycarbonate sheets and aluminum bars to prevent the leakage of propellants or combustion products. These four parts are machined accurately to a length of 29.5 inches. An igniter plate is fastened to one of the open ends with a Dash 028 (0.070-inch thick) O-ring to accommodate either ignition methods discussed in Section 3.1.3. The other open end is covered with a rupture diaphragm cut from masking tape. The adhesive on the masking tape is used to provide a partial seal on the combustor face, while a Dash 028 O-ring on the flange securing the masking tape compresses to provide an air-tight combustor. Due to safety reasons, combustion tests in tube C2 are restricted to initial pressure up to 25 psia and the diaphragm ensures relief of detonation over-pressures to protect the polycarbonate windows. Although, the chosen tube length is longer than the predicted DDT run-up distance, it is difficult to achieve DDT in this arrangement as the initial compression waves from the accelerating flame ruptures the diaphragm. This reduces the strength of the combustion wave thereby preventing DDT. A 3D schematic of tube C2 is shown in Figure 3.11. The final assembly of combustion tube C2 is shown in Figure 3.12. For reference, engineering drawings of individual parts in this assembly are included in the Appendix D.

The gas delivery system used with this combustion tube is similar to the one used with combustion tube C1. The the propellants flow into the combustion tube through two opposing ISO 11926-2 ports on the aluminum bars. The test procedure for this phase of the project is also similar to that from the high-pressure detonation experiments. The other two ISO 11926-2 ports on the aluminum bars accommodate a low-frequency pressure transducer to monitor the initial pressure of the combustible mixture and VACCON[©] fixed venturi vacuum ejector to evacuated the tube prior to propellant fill.

3.2.2 Diagnostics

The ignition process, deflagration and pre-compression in unburned gas mixture are studied using high-speed imaging. The ignition process and deflagrations are visualized using direct imaging of the events using a Photron[©] FASTCAM SA-Z camera at a frame rate of 20 kHz with a 1024×1024 pixel resolution.

To visualize the compression waves produced by the accelerating flame, a schlieren system is integrated into the high-speed imaging setup. A schematic of the schlieren system used is shown in Figure 3.13. A 3.45×3.45 mm emitter LED with a 125° wide angle and minimum luminous flux of 1300 lm is used to create an approximate point light source. The light from the LED is collimated onto the test section in tube C2 using a 3-inch diameter lens with a focal length of 13.5 inches. Downstream of the test section, the collimated light is converged onto a circular knife edge using a 3-inch diameter lens with a focal length of 9.5 inches. The schlieren images are recorded using a Photron[©] FASTCAM SA-Z camera at a frame rate of 20 kHz with a 1024×1024 pixel resolution. An exposure time of 3.75 μ s is used for most tests and is reduced to 2.50 μ s or 1.25 μ s to capture details of some fast deflagrations. The

circular knife edge, both lenses and the LED light source are removed when directly imaging the deflagration. No other instrumentation is used on this combustion tube.






Figure 3.5. Nichrome igniter. (a) Nichrome wire soldered to the leads of Kemlon[©] feed through; (b) Schlieren image of heated nichrome wire prior to ignition of combustible mixture.



Figure 3.6. Schematic of the high-energy spark discharge circuit.



Figure 3.7. Igniter adapter with spark plug. (a) Top view; (b) Front view.



Figure 3.8. Cross-section view of optic port in igniter adapter showing major components [82].



Figure 3.9. Cross-section view of igniter adapters with optic port and igniter ports. A: with port for Nichrome wire igniter; B: with port for spark plug.



Figure 3.10. System pressures during a typical test using the evacuated fill method.



Figure 3.11. 3D schematic of combustion tube C2 with labelled parts.



Figure 3.12. Assembled combustion tube C2 on the optics table with propellant lines, pressure transducer stand-off line (white plastic tube) and vacuum ejector (blue cylinder). The spark igniter is fastened to the igniter flange on the right.



Figure 3.13. Schematic of the high-speed schlieren system used to visualize deflagrations in combustion tube C2.

4. THEORETICAL CALCULATIONS

This chapter presents theoretical flame and detonation calculations. The theoretical detonation calculations will be used for comparison with experimental measurements and the flame calculations will be used to explain flame acceleration measurements in the planar detonation setup. A summary of the calculated parameters considered is this study is given in Table 4.1. The theoretical parameters are calculated for a range of initial pressures (p_0) and equivalence ratios (ϕ) using Cantera [83], an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. The parameters considered are: laminar flame speed (S_L) , expansion ratio (θ), product of laminar flame speed and expansion ratio (visual flame speed), CJ detonation pressure (P_{CJ}) and velocity (D_{CJ}) , ZND induction time (τ_i) and exothermic pulse time (τ_e) . These parameters are calculated for three fuel-oxidizer combinations: ethylene-nitrous oxide, ethylene-oxygen, and ethylene-air. Additionally, CJ detonation properties are calculated for acetylene (C_2H_2) -nitrous oxide and ethylenenitrogen tetroxide (N_2O_4) . Calculations involving ethylene-air and ethylene-nitrogen tetroxide are for benchmark comparisons. In addition to these properties, reflected pressure calculations are performed for ethylene-nitrous oxide at different initial pressures to provide a scale for reflected pressures measured in the experiments relative to CJ detonation pressures. The calculations are carried out at an initial temperature of 300 K for all cases. When varying the initial pressure, a stoichiometric equivalence ratio is used; when varying the equivalence ratio, the initial pressure is kept constant at 1 atm (14.7 psia). The thermodynamic and transport data used in these calculations is from the Mével mechanism [41] which includes relevant nitrogen and oxygen chemistry with small hydrocarbons. The following section presents detonation calculations and Section 4.2 describes flame properties in the considered mixtures.

Figure Number	Parameter	Oxidizer	Comments
4.1(a)	CJ Detonation Velocity vs. Initial Pressure	$\begin{array}{c} N_2O,O_2,\\ Air,N_2O_4 \end{array}$	T_{CJ} vs. p_0 plots follow similar trends
4.1(b)	CJ Detonation Velocity vs. ϕ	$\begin{array}{c} N_2O,O_2,\\ Air,N_2O_4 \end{array}$	D_{CJ} greatest for N ₂ O at $\phi \leq 0.4$ due to highest heat of reaction
4.2(a)	CJ Detonation Pressure vs. Initial Pressure	$\begin{array}{c} N_2O,O_2,\\ Air,N_2O_4 \end{array}$	Ranking of P_{CJ} at a given p_0 is a function of mixture molecular weight
4.2(b)	CJ Detonation Pressure vs. ϕ	$\begin{array}{c} N_2O,O_2,\\ Air,N_2O_4 \end{array}$	Plot trends are due to direct proportionality with D_{CJ}^2
4.3	Reflected & CJ Pressure vs. Initial Pressure	N ₂ O	
4.5(a)	ZND Induction Time vs. Initial Pressure	N_2O, O_2, Air	Main dependency is on ρ_s
4.5(b)	ZND Induction Time vs. ϕ	N_2O, O_2, Air	Dependent on ρ_s and fuel-oxidizer concentration
4.6(a)	ZND Exothermic Pulse Time vs. Initial Pressure	N_2O, O_2, Air	τ_{e,N_2O} comparable to τ_{e,O_2}
4.6(b)	ZND Exothermic Pulse Time vs. ϕ	N_2O, O_2, Air	τ_{e,N_2O} comparable to τ_{e,O_2}
4.7(a)	Laminar Flame Speed vs. Initial Pressure	N_2O, O_2, Air	No p_0 dependence
4.7(b)	Laminar Flame Speed vs. ϕ	N_2O, O_2, Air	Maximum at slightly rich conditions and tails off on either sides
4.8(a)	Expansion Ratio vs. Initial Pressure	N_2O, O_2, Air	Remains approximately constant with changing p_0
4.8(b)	Expansion Ratio vs. ϕ	N_2O, O_2, Air	Trends are similar to P_{CJ} vs. ϕ
4.9(a)	Visual Flame Speed vs. Initial Pressure	N_2O, O_2, Air	
4.9(b)	Visual Flame Speed vs. ϕ	N_2O, O_2, Air	

Table 4.1. Summary of theoretical calculations in this chapter.

4.1 Detonation Parameters

The detonation parameters discussed in this section are calculated using the Shock and Detonation Toolbox (SDT), an open-source software library that uses the Cantera software package [84]. It has the capability to compute both CJ and ZND detonation properties. As discussed in Chapter 1, the CJ detonation properties are obtained using purely thermodynamic calculations, while the ZND properties are 1D calculations based on reaction rates to describe the detonation structure.

4.1.1 CJ Detonation Parameters

First, the CJ detonation velocity (D_{CJ}) as functions of initial pressure (p_0) and equivalence ratio (ϕ) are shown in Figures 4.1(a) and 4.1(b). For stoichiometric mixtures of nitrous oxide, oxygen and air with ethylene, the CJ detonation velocities are highest with oxygen as the oxidizer and lowest with air, and the velocities for all three mixtures increase only slightly over the range of 14.7-350 psia initial pressures, with a relatively faster increase at lower initial pressures. These features are shown in Figure 4.1(a). The reason for this behavior is understood by looking at the simplified expression for CJ detonation velocity, Equation 1.6. The CJ detonation velocity is directly proportional to the ratio of specific heats, γ , and the square root of heat of reaction, Q, of the mixture. Assuming complete combustion, the heat of reaction is the highest for oxygen mixtures, then ethylene-nitrous oxide $(\approx 0.58Q_{O_2})$ and lowest for ethylene-air $(\approx 0.28Q_{O_2})$, but remains constant with increasing initial pressure. Therefore, the slightly increasing trend of the CJ detonation velocity curves is attributed to the variation in the ratio of specific heats with initial pressure. Although, γ is highest for air mixtures and lowest for oxygen mixtures, this difference is negligible enough (average burned equilibrium values: $\gamma_{air} = 1.23$, $\gamma_{N_2O} = 1.17$ and $\gamma_{O_2} = 1.16$) that heat of reaction is the dominant factor in driving the ranking in CJ detonation velocities for these mixtures. This is also discussed by Kaneshige et al. [12] in their work on detonations in mixtures containing nitrous oxide. They conclude that D_{CJ} of nitrous oxide mixtures is lower than that of oxygen mixtures because of the production of N_2 during the dissociation of N_2O . The N_2 dilutes the combustion products, which offsets energy release due to the positive heat of formation of N_2O . Due to this, O_2 is a more energetic oxidizer than N_2O for stoichiometric and fuel-rich mixtures. This work also compares the performance of ethylene and acetylene as a mixture with nitrous oxide. The CJ detonation velocity calculations for acetylene are comparable to ethylene, but slightly higher due to the higher heat of reaction with acetylene. The theoretical calculations also include CJ detonation velocities for ethylene-nitrogen tetroxide for benchmark comparison with the other mixtures and are again higher than those for ethylene-nitrous oxide, but lower than ethylene-oxygen.



Figure 4.1. Theoretical CJ detonation velocities for gas mixtures. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

The CJ detonation velocity as a function of equivalence ratio at a fixed initial pressure of 14.7 psia is shown in 4.1(b). An interesting trend is observed at lean equivalence ratios. At equivalence ratios $\phi \leq 0.4$, the CJ detonation velocity is higher for nitrous oxide mixtures than oxygen mixtures and this is due to the higher heat of reaction for ethylene-nitrous oxide mixtures in comparison to ethylene-oxygen mixtures in that region. For fuel lean mixtures, Kaneshige et al. [12] conclude that the decomposition of N₂O plays an essential role in making these mixtures more detonable than those with oxygen as the oxidizer. Nitrous oxide can exothermically decompose even in the absence of a fuel leading to higher detonation velocities for lean fuel-N₂O mixtures than those in fuel-O₂ mixtures at the same equivalence ratio. However, Kaneshige et al. [12] reported that for extremely lean mixtures, the N₂O decomposition is limited by the lack of H-atom bearing species which are required to catalyze the decomposition reaction. Their tests do not result in detonations in mixtures of less than 5% H₂ with N₂O.

Next, CJ detonation pressures (P_{CJ}) are compared for these five mixtures as functions of initial pressure (p_0) and equivalence ratio (ϕ) and are shown in Figures 4.2(a) and 4.2(b). For all mixtures at $\phi = 1$, P_{CJ} increases linearly with increasing initial pressure, with nitrogen tetroxide mixtures producing the highest detonation pressures, followed by nitrous oxide, oxygen and lowest for air mixtures. Once again, ethylene and acetylene with nitrous oxide produce comparable values. There is a unique slope for the CJ pressure versus initial pressure curve for each mixture: 68.42 for ethylene-N₂O₄, 42.49 for acetylene-N₂O, 41.47 for ethylene-N₂O, 36.85 for ethylene-O₂ and 19.15 for ethylene-air. With ethylene as the fuel, the increase in detonation pressure when changing from oxygen to nitrous oxide is relatively small, approximately 12-15%. Once again, analyzing this trend based on CJ theory, Equation 1.7 indicates that CJ detonation pressure is directly proportional to the unburned gas density (ρ_0) and to the square of the CJ detonation velocity (D_{CJ}). For example, scaling the CJ detonation pressures for ethylene-nitrous oxide and ethylene-oxygen mixtures with these properties leads to the following:

$$\frac{P_{CJ,N_2O}}{P_{CJ,O_2}} \sim \frac{D_{CJ,N_2O}^2}{D_{CJ,O_2}^2} \frac{\rho_{u,N_2O}}{\rho_{u,O_2}} = (0.85)(1.345) = 1.14.$$
(4.1)

This value is very close to the average ratio of CJ detonation pressures for these two mixtures (= 1.134) in the initial pressure range considered. As discussed earlier in this section, the CJ detonation velocity does not vary much with initial pressure and therefore the increasing trend in CJ detonation pressure is solely attributed to the linear increase in unburned density of the mixtures.

Assuming an ideal gas, for a given initial temperature, the unburned density is a directly proportional to the initial pressure and molecular weight of the unburned gas mixture. For each fuel-oxidizer mixture, the molecular weight of the unburned mixture at $\phi = 1$ is constant and does not change with increasing pressure. Thus, the increase in the unburned gas density is directly proportional to the increase in initial pressure, where the constant of proportionality is the molecular weight. In comparing nitrous oxide with oxygen and air, nitrous oxide mixtures have the highest molecular weights (≈ 66), then oxygen mixtures (≈ 31) and lowest for air mixtures (≈ 29). Therefore, the higher molecular weights for nitrous oxide mixtures explains the higher P_{CJ} for nitrous oxide versus oxygen mixtures.

The CJ detonation pressures as a function of equivalence ratio are shown in Figure 4.2(b). The trends are similar to the non-linear dependence of CJ detonation velocities on ϕ shown previously in Figure 4.1(b). This is explained by the fact that the unburned gas densities of these mixtures are relatively constant over the selected range of equivalence ratios and hence they only act as scaling factors in the equation for CJ detonation pressure. Due to this scaling, higher densities of nitrous oxide mixtures over oxygen mixtures, due to higher molecular weights, produce higher CJ detonation pressures.



Figure 4.2. Theoretical CJ detonation pressures for gas mixtures. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

Calculations of reflected detonations are also performed for comparison with the recorded pressures at the closed end of the combustion tube (p_{13}) . The theoretical reflected detonation pressure vs. initial pressure for a stoichiometric ethylene-nitrous oxide mixtures is shown in Figure 4.3. The reflected detonation pressure is approximately 2.5 times larger than CJ detonation pressure for the same initial pressure,

as expected from basic reflected shock theory. However, these calculated reflected pressures are still significantly lower than the measured pressures at the reflecting end (p_{13}) , as discussed in the following chapter.



Figure 4.3. Comparison of theoretical CJ detonation and reflected detonation pressures for stoichiometric ethylene-nitrous oxide vs. initial pressure.

4.1.2 ZND Parameters

As discussed in Chapter 1, a detonation is a supersonic combustion wave in which the leading shock and reaction zone are coupled. The leading shock raises the temperature and pressure of a combustible mixture initiating a coupled thermal chainbranching explosion. After an induction time, exothermic recombination reactions create product species whose expansion acts as a piston propelling the shock wave forward. The interaction between the leading shock and consequent reaction zone is a defining characteristic of self-sustained detonations [85]. The basic features of this detonation structure are captured in the ZND model. A schematic representation of the ZND detonation structure in shock-fixed coordinates is shown in Figure 1.3. This model assumes that the mixture composition remains the same across the leading shock. The region behind the shock is defined by two time scales: τ_i , the induction time, and τ_e , the exothermic pulse time. These time scales are determined from the thermicity profile in the region behind the leading shock. An example of a thermicity profile is shown in Figure 4.4 obtained from ZND calculations for a stoichiometric ethylene-oxygen mixture at 70 psia. The time scales are calculated using the ZND solver in the Shock and Detonation Toolbox [84] in Cantera [83]. For ease of comparison, the ZND calculations presented in this chapter are restricted to ethylene-nitrous oxide, ethylene-oxygen and ethylene-air mixtures only.



Figure 4.4. Example of a thermicity profile behind the leading shock of the ZND structure for stoichiometric ethylene-oxygen at 70 psia and 300 K.

The induction time is the time to maximum thermicity as indicated in Figure 4.4. For the three ethylene-oxidizer mixtures, these times are calculated at stoichiometric equivalence ratio with increasing initial pressure, shown in Figure 4.5(a), and at 14.7 psia (1 atm) initial pressure with varying equivalence ratio, shown in Figure 4.5(b). The figures provide a relative comparison of the time duration over which chain branching reactions occur. For all initial pressures and equivalence ratios, oxygen mixtures have the shortest induction times with air mixtures having the longest times. As shown in Equation 1.10, induction time is a function of the post-shock density and temperature and the activation energy. From calculations, it is seen that the term $exp\left(\frac{E_a}{RT_s}\right)$ does not vary appreciably with initial pressure for oxygen and air mixtures, but increases three times for nitrous oxide mixtures (N₂O: 0.5 - 1.5, O₂: 0.011 - 0.016 and Air: 0.13-0.16). The post-shock density increases with increasing initial pressure for all ethylene-oxidizer mixtures, with the highest increase for nitrous oxide mixtures and lowest for air mixtures and this is due to the difference in molecular weights of the mixtures as discussed in Section 4.1.1. Therefore, τ_i decreases at a rate of $1/\rho_s^2$ for oxygen and air mixtures, but for nitrous oxide mixtures τ_i decreases slower than $1/\rho_s^2$ as $exp\left(\frac{E_a}{RT_s}\right)$ is increasing with increasing p_0 . This inverse square proportionality of τ_i to ρ_s leads to the shape of the curves shown in Figure 4.5(a). In addition to these dependencies on the initial pressure, τ_i is also inversely proportional to fuel and oxidizer concentrations, and the varying reactant concentrations due to increasing ϕ is responsible for the trends shown in the figure 4.5(b).



Figure 4.5. ZND induction time for gas mixtures with ethylene. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

Next, the exothermic recombination zone is characterized by the exothermic pulse time and is defined as the full-width at half-maximum of the thermicity pulse as shown in Figure 4.4. The exothermic pulse time is calculated for the same initial conditions as those used for the induction time and plotted in Figures 4.6(a) and 4.6(b). These times are comparable for the nitrous oxide and oxygen mixtures at equivalence ratios above 0.5 for all initial pressures, but τ_e for air mixtures are at least an order magnitude higher. Effectively, the rate of heat release in the reaction zone with nitrous oxide as the oxidizer is comparable to that in a fuel-oxygen mixture.



Figure 4.6. ZND exothermic pulse time for gas mixtures with ethylene. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

4.2 Flame Parameters

A study on deflagration-to-detonation transition is not complete without the understanding of the accelerating flame and the flame properties which affect this acceleration. Consider a flame initiated at the closed end of a vessel and propagating towards the opposite end, inducing an outward flow in the unburned gas mixture ahead of it due to expansion of the high temperature burned gases. Considering a 1D assumption, this induced flow has a velocity $u = (\theta - 1)S_L$ while the flame propagates with a velocity $U_{fL} = \theta S_L$ in the laboratory frame of reference [86], where S_L is the normal laminar flame speed at the ambient conditions and $\theta = \rho_u/\rho_b$ is the expansion ratio or the ratio of unburned to burned gas densities. The flame front moves with laminar flame speed, S_L with respect to the upstream flow and simultaneously is entrained by the flow ahead of it with its local velocity. Due to friction at the walls, the flame front moves slower near the walls in comparison to the axis of the vessel. This establishes a finger-shaped flame front and the flame front is stretched as it advances into the unburned flow ahead. The stretching of the flame front increases the rate of heat release which enhances the effective burning velocity. An increased burning velocity further induces the flow field ahead of the flame which leads to further flame stretching. Due to this positive feedback, the velocity of the combustion wave during early stages increases exponentially in time as

$$U_{fL} = \theta S_L exp(\alpha S_L t/d), \qquad (4.2)$$

where α is a numerical factor of the order of unity [21].

In order to achieve deflagration-to-detonation transition in a mixture, an essential preceding phenomenon is acceleration of the flame. Therefore, empirical correlations and simplified analytical models to predict run-up distance have been derived based on the flame parameters that are important for acceleration. For example, some of these parameters are laminar flame speed, expansion ratio which is directly related to the heat of combustion, and the velocity or Reynolds number of the induced flow in the unburned gas. These analytical models also assume that the flame must accelerate to a critical speed, equal to the speed of sound in the unburned gases, in order to transition to a detonation. So, Bollinger et al. [15] develop such an empirical correlation based on the heat of combustion, laminar flame speed, sonic velocity in the unburned mixture (a_u) and Reynolds number (Re_u) of the induced flow in the unburned mixture by the expansion of the burned gases. The heat of combustion is accounted for as the ratio of flame temperature to initial temperature (T_b/T_u) . They also discuss that a mixture with a fast burning speed can induce a sufficiently high Reynolds number to induce turbulence in unburned mixture. They use the Reynolds number of the unburned gas flow, based on the laminar flame speed and tube diameter, to establish a qualitative relationship between flame turbulence and the detonation run-up distance. Based on these parameters they develop an empirically determined K function

$$K = Re_u \left(\frac{S_L}{a_u}\right) \left(\frac{T_b}{T_u}\right) \tag{4.3}$$

and plot the measured run-up distances for CO-O_2 , H_2 - O_2 and CH_4 - O_2 as a function of K. A unique trend is observed between the measured run-up distances and the Kfunction for the H_2 - O_2 and CO-O_2 systems irrespective of the initial pressure or fuel concentration. However, for the stoichiometric CH_4 - O_2 and 50% CH_4 - O_2 systems, the trends followed by the data points are shifted away from the earlier trend, with the latter system significantly separated from the others reported in this study.

It is possible that the results from the ethylene-oxidizer tests in the current work could be correlated with parameters in the combustion wave velocity relation or the K function. might follow the combustion wave velocity relation (Equation 4.2) or agree with the K function correlation (Equation 4.3). These models are based on the laminar flame speed and expansion ratio of the combustible mixture, so it is essential to understand the behavior of these properties at different initial conditions. By definition, the laminar flame speed of a mixture, S_L , is the velocity at which a flame propagates orthogonally into a quiescent mixture [3]. The laminar flame speeds are calculated for all three ethylene-oxidizer mixtures as functions of initial pressure and equivalence ratio and are shown in Figures 4.7(a) and 4.7(b). The laminar flame speed of ethylene-oxygen is the highest for all initial conditions and has a weak positive dependence on initial pressure. The laminar flame speeds for nitrous oxide and oxygen mixtures remain approximately constant over the considered range of initial pressures. With a variation in equivalence ratio, all three systems exhibit peaks in laminar flame speeds around the stoichiometric mixture ratio as expected. The lack of pressure dependence of laminar flame speeds is in accordance with the theory of Mallard and Le Châtelier, which states that

$$S_L \sim p^{(n-2)/2}$$
 (4.4)

where n is the global reaction order [87] and is approximately equal to 2 for the three mixtures.



Figure 4.7. Laminar flame speed for gas mixtures with ethylene. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

Another important parameter influencing the early stages of flame acceleration is the expansion ratio, θ , which is the ratio of densities in the unburned (ρ_u) to the burned mixture (ρ_b). The expansion ratios are calculated for the mixtures in this study across an isobaric flame and are shown in Figures 4.8(a) and 4.8(b). The unburned gas density is directly proportional to the initial pressure and molecular weight of the mixture, and for a given initial pressure, the unburned density is highest for the nitrous oxide mixtures due to its high molecular weight and lowest for air mixtures. The unburned molecular weights do not vary as a function of initial pressure which results in a linear dependence of unburned gas density on initial pressure. The burned gas density is again directly proportional to the molecular weight and pressure of the burned gas, and inversely proportional to the flame temperature. The burned molecular weight and flame temperature increase slightly with increasing initial pressure which again results in a linear dependence of burned density on initial pressure of gas mixture. Due to this, there is no appreciable variation in the expansion ratio of these mixtures with increasing initial pressure, resulting in $\theta_{N_2O} \approx 17$, $\theta_{O_2} \approx$ 15 and $\theta_{air} \approx 8.2$. However, varying the mixture ratio changes the molecular weight of the burned gas and the flame temperature, resulting in the shape of expansion ratio curves as a function of equivalence ratio shown in Figure 4.8(b).



Figure 4.8. Expansion ratio for gas mixtures with ethylene. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

In the early stages of burning in a closed vessel, the velocity of the flame increases due to confinement of the combustion products. As mentioned earlier, considering a 1D assumption, the visual flame speed of the combustion wave (U_{fL}) increases exponentially from an initial value of θS_L with time. In this initial phase of propagation, the velocity of the flame is related to this product of laminar flame speed and expansion ratio as described in Equation 4.2. The expansion ratio amplifies the laminar flame speed and the variation in visual flame speeds are shown in Figures 4.9(a) and 4.9(b) for the different mixtures. Nettleson reports that an analysis of flame acceleration indicates that a shock first forms as the velocity of the flame approaches the speed of sound in the uncompressed reactants [3]. Thus, a mixture with a higher initial visual flame speed and laminar flame speed exhibits faster flame acceleration which can lead to earlier DDT.



Figure 4.9. Visual flame speeds for gas mixtures with ethylene. (a) vs. initial pressure at $\phi = 1$; (b) vs. ϕ at 14.7 psia (1 atm) initial pressure.

5. EXPERIMENTAL RESULTS & DISCUSSION

5.1 Data Analysis Methods

For all tests conducted in combustion tube C1, the main measurement parameters are pressure induced by the combustion wave during its propagation, light intensity from the combustion, and pressure and temperature upstream of the the sonic venturis on the propellant lines. General details of the methods used to analyze the data from these measurements are discussed in this section. More specific details of these methods are discussed along with the results.

5.1.1 Mixture Ratio

The pressures (P_u) and temperatures (T) upstream of the sonic venturis are sampled at 100 Hz each and are recorded using a National Instruments[©] USB-6351 data acquisition module via LabVIEW software. These pressure and temperature measurements are used to monitor the progress of tests and to calculate the mass flow rate (\dot{m}) of the gases introduced into the combustion tube. The venturis remain choked for a steady upstream pressure at least 1.2 times the downstream pressure and thus maintains a constant mass flow rate. In these tests, an upstream pressure at least 1.35 times the target mixture pressure in the combustion tube is maintained on both propellant lines to ensure choked flow through the sonic venturis during the entire fill period. The propellant delivery lines are designed such that the volume between the pneumatic valve and the sonic venturi is sufficiently small that the pressure rises to a steady upstream pressure instantaneously upon actuating the valve, with negligible transient behavior in the mass flow rate. Using this property of a sonic venturi and assuming ideal gas behavior, the mass flow rate of each gas is calculated as:

$$\dot{m} = \frac{C_d A_s P_u}{\sqrt{\frac{R_u T}{\mu g}}} \sqrt{\left(\gamma \frac{2}{\gamma + 1}\right)^{\frac{\gamma + 1}{\gamma - 1}}}.$$
(5.1)

The actual O/F ratio is then calculated as the ratio of oxidizer mass flow rate to fuel mass flow rate. The sonic venturis are designed and manufactured by $FlowMaxx^{T}$ Engineering in accordance with ASME MFC-7M standards, which predicts an uncalibrated flow accuracy of $\pm 1\%$ of flow reading. The actual O/F ratio for all tests, based on this method of setting mass flow rates using sonic venturis, is within 10% of the targeted stoichiometric O/F ratio.

5.1.2 Combustion Pressure

As discussed in Chapter 3, 10 PCB[®] 109C11 pressure transducers are installed along the length of combustion tube C1. The first pressure transducer is located 4.378 inches away from the igniter plane and the subsequent transducers are 6 inches apart. The last transducer on the tube side wall and the one at the dead end are 4.65 inches apart. These high-frequency pressure transducers are sampled at 600 kHz each and the signals from these transducers recorded during a typical test are shown in Figure 5.1.

The amplitude corresponding to the first peak of each pressure signal is chosen as the pressure at that pressure transducer location. At least four tests are conducted at each initial pressure to assess the repeatability of measured pressures. These multiple tests at each initial pressure provide a recording of at least four peak pressures at each pressure transducer location along the tube. At each pressure transducer location, the multiple peak pressures measured are averaged to provide a representative mean peak pressure at that location and the associated standard deviation is also calculated. Post-DDT, these mean peak pressures show some variation along the tube, which is shown in Figure 5.2 for ethylene-N₂O at 20 psia initial pressure using spark ignition.



Figure 5.1. Pressure signals from a typical test for a stoichiometric ethylene-nitrous oxide mixture at $p_0 = 50$ psia.

The error bars in Figure 5.2 represent the standard deviation of the measured peak pressures at each location, which corresponds to the variation in peak pressures.



Figure 5.2. Mean peak pressure at each location along the combustion tube and standard deviation of peak pressures over multiple tests with C_2H_4 -N₂O at $p_0 = 20$ psia using spark ignition. CJ pressure is represented by the dashed line. No pressure transducer at locations 9 & 11.

The sensor surface on the PCB[®] pressure transducers has a diameter of 0.245 inches and are installed in a recessed configuration as shown in the schematic in Figure 5.3. The recess protects the sensing surface from the harsh combustion envi-

ronment and a reduced recess diameter relative to that of the sensing surface improves spatial resolution of the measurement. The recess diameter used on all ports is 0.188 inches, but this dimension is a few orders of magnitude larger than the detonation reaction zone thickness. Due to this, these pressure transducers cannot measure the post-shock von Neumann spike described in Chapter 1 as the detonation pressure profile is averaged over the recess diameter. As a consequence of this, the measured pressure is much closer to the equilibrium pressure of the detonation wave as highlighted by Craven and Greig [88]. This discussion is important in understanding that the peak pressures measured in this work, although higher than CJ detonation pressures, are certainly not the von Neumann spikes.



Figure 5.3. Schematic of the PCB[®] pressure transducer port on combustion tube C1 with details of the recess depth.

A consequence of installing these pressure transducers in a recess port is the attenuation/amplification and phase distortion of the measured pressure signal. A preliminary study on the effects of PCB[®] transducer installation port design on pressure signals is included in Appendix B. Although this study provides some insight into the difference between steep-fronted pressures measured by a pressure transducer installed in a flush versus recessed port, the calibration resulting from these measure-

ments is not used to correct the pressures measured in the nitrous oxide detonation study. This is due to the complex behavior of steep-fronted pressure waves in reactive flows and their dependence on several initial conditions such as pressure, temperature, propellant combination and mixture ratio, to name a few.

5.1.3 Combustion Velocity

In addition to pressure measurements, consecutive pressure signals are crosscorrelated to obtain the time delay between them. The distance between consecutive pressure transducers is then divided by this time delay to determine the average velocity of the combustion wave between these pressure transducers. These velocities along the tube are shown in Figure 5.4 at half-point locations to indicate that they are average velocities between two consecutive measurement locations. The error bars again indicate variations in the velocity at each location over multiple tests conducted at an initial pressure and Figure 5.4 shows that these variations are minimal post-DDT.



Figure 5.4. Average velocity at each location along the combustion tube and standard deviation of velocities over multiple tests with C_2H_4 -N₂O at $p_0 = 20$ psia. CJ velocity is represented by the dashed line. No pressure transducer at locations 9 & 11.

The velocity profile shown in Figure 5.4 can be used to estimate the location of DDT. For the case shown in Figure 5.4 (ethylene-N₂O at $p_0 = 20$ psia), the deflagration transitions to a detonation in the region between pressure transducers 3 and

4 because the interpolated combustion wave velocity exceeds the CJ detonation velocity. This method of estimating the DDT location or run-up distance is usually referred to as the time of flight (TOF) method, which has been used in an earlier series of tests [54] and by other researchers with photodiodes [19,89], ion probes [90] or pressure transducers [18,20,79,89,91] along the combustion tube. However, since the estimated velocity is an average of the velocity between two consecutive locations, it is more likely that the DDT location for the case in Figure 5.4 is somewhere between transducer locations 2 and 3.

5.1.4 Run-up Distance

To determine the DDT location and measure the run-up distance with better accuracy, the PMT module installed axially at the ignition plane is used to measure the light intensity of the combustion wave. As described in Chapter 3, the light intensity suddenly increases when the deflagration transitions to a detonation. Figure 5.5 shows an example of the PMT signal and the time associated with the circled inflection point represents the DDT time (t_{DDT}) .

The deflagration is said to have transitioned to a detonation beyond t_{DDT} and travels at a stable velocity. On a distance-time plot, this stable velocity is the slope of the straight line representing the detonation trajectory. Such a distance-time plot is shown in Figure 5.6, where the pressure signals and the PMT signal are also superimposed to determine the DDT location. This is achieved by extrapolating the detonation trajectory backwards to meet the PMT signal at t_{DDT} , as shown in Figure 5.6, where the slope of the PMT signal is 2.01×10^5 V/s. The corresponding distance of this intersection from the ignition plane is defined as DDT location (L_{DDT}).

5.1.5 Pre-compression

In addition to the PCB[®] dynamic pressure transducers, two piezoresistive pressure transducers are installed in plane with the first two PCB[®] transducers closest



Figure 5.5. Signal from the PMT module installed axially in combustion tube C1. The sudden increase in the signal indicates DDT location.

to the ignition plane. These two installation planes are 4.378 and 10.378 inches from the ignition plane. The details of these sensors and their arrangement in tube C1 are described in Chapter 3. The piezoresistive pressure transducers, manufactured by Kulite[®], are used to measure and study the pre-compression caused by the accelerating flame in the unburned gas mixture ahead of it. The construction of these sensors are different from the PCB[®] sensors such that they have a protective screen called the "B" screen to eliminate the possibility of particles hitting the sensor diaphragm. The screen is 0.005 inches in front of the diaphragm and has 0.006-in holes to enable the interaction of the diaphragm with the pressure waves. So, the cavity created between the screen and the diaphragm attenuates the high-frequency content of a steep-fronted wave such as a detonation. Due to this, these pressure transducers are not able to resolve the peak pressure of a detonation wave. However, since they are DC coupled sensors with a large discharge time constant, they are well-suited to measure quasi-steady state pressures in a flow.



Figure 5.6. Distance-time plot of the combustion wave for ethylene-O₂ at $p_0 = 30$ psia showing DDT time and location. DDT location is determined at the intersection of the PMT signal and the detonation wave trajectory.

These Kulite[®] senors are installed 4.378 and 10.378 inches from the ignition plane because the flame transitions to a detonation only beyond this length in the mixtures and initial pressures investigated in this work. This enables the measurement of the compression waves produced by the accelerating flame. Similar to the PCB[®] sensors, the Kulite[®] pressure transducers are also sampled at 600 kHz each and record pressure-time signals at two discrete locations. An example of the pressure signals from these sensors is shown in Figure 5.7. For clarity, Figure 5.7 does not include the pressure signals from the PCB[®] sensors and only shows the pressure peaks from the first four PCB[®] senors as markers to reference the time of arrival of the combustion wave in relation to the Kulite[®] pressure signals. The vertical black dashed line indicates the time of DDT. This figure helps to illustrate the pressure growth in the unburned gas mixture ahead of the flame. From these pressure signals, the time at which a pressure reaches the two Kulite[®] sensors is used to estimate the distance-time path of the accelerating flame. For instance, in Figure 5.7, a compression wave with pressure p_1 arrives at the locations of the two sensors at times $t_{1,k1}$ and $t_{1,k2}$ and this forms a C+ characteristics as per 1D unsteady gas dynamics theory. Using similar information from other compression waves, like p_2 in Figure 5.7, the path travelled by the flame prior to DDT can be estimated. This analysis is further elaborated in Section 5.5.



Figure 5.7. Kulite[®] pressure signals indicating compression waves produced by the accelerating flame in a stoichiometric ethylenenitrous oxide mixture at $p_0 = 20$ psia. Temporal location of DDT is shown as a vertical black dashed line. Red markers represent the pressure peaks measured by PCB[®] pressure transducers. Red dashed lines temporally locate two compression waves of $p_1 = 10$ psia and $p_2 = 50$ psia which are used to estimate the flame path.

5.2 Detonations in Nitrous Oxide Mixtures in Combustion Tube C0 (L/d = 6.13) [6]

As mentioned in Chapter 3, the design of combustion tube C1 is motivated by tests conducted in an earlier combustion tube of L/d = 6.13 using a stoichiometric mixture of ethylene-nitrous oxide. This section briefly describes results from tests conducted in this smaller combustion tube.

Combustion tube C0 has an internal length of 24.5 inches, wall thickness of 2 inches, inner diameter of 4 inches and is constructed of alloy steel (4340). The tube is designed for a static pressure of 20 ksia and is hydrostatically tested to 30 ksia. As shown in the cross-section view in Figure 5.8, the tube has three ports on the side wall and one port through the cover (labeled 1 in Figure 5.8) which accommodate four PCB[®] 109C11 pressure transducers. The propellant delivery system and test procedures are the same as those used with combustion tube C1 except the filling procedure. A purge fill method is used for all tests in this combustion tube, which first involves purging the tube with the oxidizer for approximately 20 s to eliminate air or residual combustion gases after which the tube is allowed to equalize to ambient pressure. Then, the combustion tube is closed before fuel and oxidizer are flowed simultaneously from opposite ports to fill the rest of the volume to achieve a stoichiometric mixture. However, this method did not adequately prevent the mixing of nitrogen from purging or air with the combustible mixture. This is determined based on preliminary tests conducted in combustion tube C1 with ethylene- N_2O and ethylene- O_2 using this purge fill method. In these preliminary tests, a mixture of ethylene-O₂ did not ignite with both ignition methods below $p_0 = 50$ psia in spite of evidence from literature to prove otherwise. However, switching to the fill procedure described in Chapter 3 ensured ignition of ethylene-O₂ even at $p_0 = 14.5$ psia which leads to the conclusion that the oxidizer is diluted during the time when the tube is allowed to equalize with ambient pressure. Hence, the fill method described in Chapter 3 is used for all tests conducted in tube C1 and presented in this chapter. Ignition in C0 is achieved using a 3.5 inch nichrome wire attached to electrodes installed at locations indicated in Figure 5.8 that is energized using an 18 VDC Li-Po battery switched on by a solid state relay.



Figure 5.8. Cross-sectional view of combustion tube C0 (L/d = 6.13) with important dimensions, inlet and outlet ports and electrode locations shown

Experimental runs with initial pressures of 125, 150, 200 and 337 psia are conducted and pressure signals are recorded at four different locations along the length of the tube. The equivalence ratios achieved during these tests is within $\pm 6\%$ of the targeted stoichiometric equivalence ratio. The measured peak pressures and estimated velocities are plotted against transducer locations and shown in Figures 5.9(a) and 5.9(b). The CJ detonation pressures, P_{CJ} , and velocities, D_{CJ} , calculated using the Shock and Detonation Toolbox, are also shown in the form of ranges in these figures. The sudden rise in the peak pressure observed in Figure 5.9(a) indicates that the combustion wave has already transitioned to a detonation at this location. This behavior is observed at location 1 during all the tests presented.

The most striking result is the very high pressures recorded during the tests. For the experiment with the lowest initial pressure of 125 psia, the predicted CJ detonation pressure is approximately 5 ksia. However, the first transducer measures



Figure 5.9. Measured combustion properties in combustion tube C0 vs. transducer location. (a) Peak pressure; (b) Velocity.

a pressure more than twice the CJ value, 12.6 ksia. Similar results are also observed for the tests at higher initial pressures, with the measured peak pressure at the first transducer exceeding the predicted CJ value by a factor of 2 to 3. It is to be pointed out that these pressures are not corrected based on the recessed transducer port design as the port design is slightly different from the one used on C1. However, the average velocity of the combustion wave between the igniter and the first transducer is on the order of 90 m/s, well below the CJ detonation velocity. The heated nichrome wire ignites the gas thermally and does not produce a shock, which is necessary to directly initiate a detonation. Since the energy of the igniter is far too low to directly initiate a detonation, it must first initiate a deflagration that then transitions to a detonation between the ignition point and the first transducer.

The ethylene-nitrous oxide mixture at elevated pressures is likely highly unstable and becomes a turbulent flame immediately following ignition. The turbulent flame produces pressure waves upstream which pre-compress the unburned gas. These waves reflect off the tube walls and further interact with the flame front, magnifying the flame front turbulence and enhancing the flame acceleration. As explained by Lee [2], if the flame acceleration mechanisms can bring the flame to a critical deflagration speed (usually on the order of half the CJ speed), the flame velocity then accelerates rapidly and the flame undergoes transition to detonation. Depending on the initial flame velocity, DDT can spontaneously occur within a couple of tube diameters [2]. The first transducer on the combustion tube is loaded at a distance of 2.81 inches from the nichrome wire. During each test the flame transitions to a detonation within this distance which is approximately 0.7 tube diameters. This is an extremely short distance for DDT to occur, so the combined effects of the inherent instability of the mixture, the high initial pressure, and the flame confinement must promote extremely rapid flame acceleration.

The pressure changes moderately at the second and third transducers, but the average combustion wave speed is significantly higher than at location 1, and in most cases greater than the CJ velocity. This suggests that the detonation is overdriven in this region. As the propagating deflagration front interacts with the reflected pressure waves in the vessel, the gas near the front is continuously compressed and heated, which results in a localized explosion directly in front of the flame. This explosion creates a shock wave that has a velocity significantly higher than a CJ detonation; as the detonation forms from the shock wave, it will initially be overdriven. Therefore, we postulate that in these experiments there occurs one or more localized explosions near the deflagration front that result in an overdriven detonation wave. This also explains the extremely high pressures, as even a small overdrive factor results in a dramatic increase in the detonation pressure. Detonations are also very unstable, and this is further demonstrated by the significant variation in the pressures from one transducer to the next and also between tests at the same initial pressure, as with the two tests at 200 psia. Such large variation in the pressure is not unexpected, and the transition from deflagration to detonation is a complex phenomenon with a certain amount of variation observed in the location of transition.

Finally, the fourth pressure transducer measures the reflected detonation pressure at the end of the tube. If the detonation reaching the end wall is in fact still overdriven, then the reflected pressures measured by the transducer are consistent with what the theory predicts. From the experiments conducted thus far, it appears that the high initial pressure, sensitivity of the flammable mixture, and the high level of confinement in the tube result in nearly immediate DDT and a highly unstable, overdriven detonation reflecting from the end wall. According to Lee [2], the overdriven detonation decays in time to either a stable CJ detonation or an unstable detonation with a velocity oscillating around the CJ velocity. A glimpse of this decay is seen in the velocity plots in Figure 5.9(b) and it is possible that the detonation stabilizes at the CJ detonation velocity if the tube is long enough.

5.3 Detonations in Nitrous Oxide Mixtures in Combustion Tube C1 (L/d = 68)

A very large number of experiments are conducted in combustion tube C1 to measure detonation properties of three mixtures of interest: ethylene-nitrous oxide, ethylene-oxygen and acetylene-nitrous oxide. A summary of these tests is given in Table 5.1. A minimum of four tests are performed at each initial pressure to assess repeatability of measured properties. Tests 1 - 218 are not included in the present discussion as they are tests from the developmental phase of the experiment involving less instrumentation, imprecise propellant fill processes, TOF method of run-up distance measurement and air as the oxidizer (mixture did not ignite). The original fill method does not involve evacuating the combustion tube prior to filling with the propellants and results in the mixing of air or residual combustion products with the filled propellants. This increases the uncertainty in the equivalence ratio of the combustible mixture and hence is improved starting with Test 219. Some tests using this earlier fill method also involve initial pressures greater than 70 psia and up to 150 psia, but they do not provide any useful information regarding the dependence of flame acceleration on initial pressure and so are not useful in the present discussion. On a typical test day, an average of 12 tests can be conducted which includes time in between consecutive tests to purge the combustion tube of combustion products and to review the acquired data. Tests with the nichrome ignition method take longer to set up as the feed through with the nichrome bridge has to be replaced after every test. The measured detonation properties enable the comparison of nitrous oxide and oxygen performance, spark and nichrome ignition methods, and ethylene and acetylene performance.

Mixture	Spark Ignition	Nichrome Ignition
Ethylene- Nitrous Oxide	$p_0 = 20 - 70$ psia (1.38 - 4.83 bar) Test no.: 219 - 243 (Detonation properties), 359 - 370 (Pre-compression)	$p_0 = 20 - 70$ psia (1.38 - 4.83 bar) Test no.: 305 - 328
Ethylene-	$p_0 = 14.5 - 70 \text{ psia} (1.00 - 4.83 \text{ bar})$	$p_0 = 20 - 70 \text{ psia} (1.38 - 4.83 \text{ bar})$
Oxygen	Test no.: 244 - 253, 264 - 288	Test no.: 334 - 358
Acetylene-	$p_0 = 15 - 20$ psia (1.03 - 1.38 bar)	Did not conduct
Nitrous Oxide	Test no.: 292 - 299	

Table 5.1. Summary of tests conducted in combustion tube C1.

5.3.1 Nitrous Oxide Versus Oxygen (with C_2H_4)

One of the objectives of this work is to compare the performance of nitrous oxide with a more typical oxidizer, and so oxygen is chosen for this purpose. Mixtures of ethylene-N₂O and ethylene-O₂ are tested at initial pressures (p_0) ranging from 20 - 70 psia in increments of 10 psia in combustion tube C1 using both ignition methods. Additionally, ethylene-O₂ is also tested at an initial pressure of 14.5 psia with spark ignition. Ignition is achieved in all mixtures and transition to a detonation is observed at all investigated initial pressures. CJ detonation calculations discussed in Chapter 4 indicate that ethylene-O₂ results in higher detonation velocities, whereas ethylene-N₂O produces higher detonation pressures. A comparison of the distribution of peak pressures along the length of C1 between ethylene-N₂O and ethylene-O₂ is shown in Figure 5.10 for $p_0 = 20$ psia as an example. As a reminder, the marker at each pressure transducer location in Figure 5.10 is an average of the peak pressures measured at that location over at least four tests with the same initial pressure. Figure 5.10 shows that the peak pressures are higher for ethylene-N₂O, as predicted from CJ theory, at all locations except at locations 1 and 12. The comparable peak pressures and overlapping error bars at location 12 for these two mixtures is possibly just a coincidence. However, the lower peak pressure at location 1 for ethylene-N₂O is a consequence of slower flame acceleration in this mixture in comparison to ethylene-O₂. Due to this, at location 1, the combustion wave in ethylene-O₂ has already transitioned to a detonation, but the combustion wave in ethylene-N₂O is still a fast deflagration resulting in peak pressures lower than the CJ detonation pressure for this mixture. For reference, the CJ detonation pressures for these mixtures at $p_0 =$ 20 psia are also shown in the same figure.



Figure 5.10. Comparison of C_2H_4 -N₂O and C_2H_4 -O₂ peak pressures at $p_0 = 20$ psia. Also, includes comparison of $p_0 = 20$ and 40 psia C_2H_4 -N₂O peak pressures. Tests shown here use spark ignition (S) and error bars indicate variation in measured peak pressure at that location. No pressure transducer at locations 9 & 11.

Evidence of this behavior is also highlighted in a comparison of velocity distribution of the combustion wave along the tube for these two mixtures in Figure 5.11. CJ detonation velocities are not shown in Figure 5.11 to reduce clutter, but the combustion wave is considered to have transitioned to a detonation when the velocity does not change appreciably. Using this criteria, Figure 5.11 shows that the deflagration accelerates slower to a detonation in C_2H_4 - N_2O over C_2H_4 - O_2 at $p_0 = 20$ psia. This explains the lower peak pressure in C_2H_4 - N_2O at location 1 in comparison to that in C_2H_4 - O_2 . The large error bars at location 1.5 for C_2H_4 - O_2 and location 2.5
for C_2H_4 -N₂O are indicative of fluctuations in the estimated average velocities due to the occurrence of deflagration-to-detonation transition (DDT) at these locations. During DDT, the combustion wave is overdriven due to the explosion of compressed unburned gases between the precursor shock and reaction zone [3] and this event is not very repeatable, thereby causing a fluctuation in the estimated velocity around the DDT location.



Figure 5.11. Comparison of C_2H_4 -N₂O and C_2H_4 -O₂ average velocities at $p_0 = 20$ psia. Also, includes comparison of $p_0 = 20$ and 40 psia C_2H_4 -N₂O average velocities. Estimated velocities are for the tests shown in Figure 5.10. Error bars indicate variation in estimated velocity at that location.

Figures 5.10 and 5.11 also compare the pressure and velocity distribution along the combustion tube for C_2H_4 -N₂O at two different initial pressures, 20 and 40 psia. As predicted by CJ theory, the combustion pressures at all locations for $p_0 = 40$ psia are either greater than or comparable to those for $p_0 = 20$ psia. Peak pressures are comparable between these two initial pressures at locations 3 and 4, due to the overdriven nature of the combustion wave for $p_0 = 20$ psia causing elevated detonation pressures. The deflagration also accelerates faster to a detonation at the higher initial pressure, as shown in Figure 5.11, indicating that the run-up distance to detonation decreases with an increase in initial pressure.

In order to study the dependence of detonation pressure on initial pressure for the mixtures investigated in this work, the recorded peak pressures along the tube from multiple tests are analyzed and a representative average detonation pressure is computed. The method used to compute this average detonation pressure and the associated standard deviation for each mixture and initial pressure is shown in Figure 5.12 for C₂H₄-N₂O at $p_0 = 20$ psia as an example. In this method, the mean of peak pressures from all locations in the post-DDT regime of the propagating flame from multiple tests at an initial pressure, p_0 , is computed to be the average detonation pressure, P_{p_0} . Mathematically, this is represented as

$$P_{p_0} = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} (p_{i,j} \ge P_{CJ})$$
(5.2)

where, $p_{i,j}$ is the peak pressure from i^{th} test and j^{th} location. The standard deviation, represented by error bars, is computed using the same criteria of peak pressure selection.



Figure 5.12. Illustration of the method used to compute a representative average detonation pressure over multiple tests at a given initial pressure. Illustration is shown here for C_2H_4 -N₂O at $p_0 = 20$ psia (Tests 219 - 222).

These average detonation pressures and standard deviations are plotted against initial pressure (p_0) in Figure 5.13 for C_2H_4 - N_2O and C_2H_4 - O_2 tests using spark ignition (S). Consistent with the ranking predicted by the theoretical CJ calculations, average detonation pressures are lower for ethylene- O_2 . On an average, they are lower by 31% in comparison to the average detonation pressures of ethylene-N₂O. The second observation is that the measured detonation pressures for both mixtures at all initial pressures are higher than the calculated CJ detonation pressures as shown in Figure 5.13. This is due to the pre-compression of the unburned gas mixture prior to DDT. This phenomenon is discussed further in Section 5.5. Finally, on comparing the standard deviations of peak pressures for nitrous oxide and oxygen mixtures in Figure 5.13, nitrous oxide tests have larger standard deviations than those from oxygen mixtures, suggesting larger pressure oscillations with nitrous oxide as the oxidizer. In addition to being an oxidizer, nitrous oxide is a monopropellant, which exothermically decomposes at elevated temperatures. Thus, when ethylene- N_2O detonates, it is likely that the compression heating causes nitrous oxide to explode unassisted (without reaction with ethylene), which manifests as large pressure oscillations rendering the detonation unstable.

The average detonation velocities for these two mixtures are plotted against initial pressure (p_0) in Figure 5.14. Similar to the criteria used for the selection of peak pressures to compute a representative detonation pressure, a criteria of selecting measured velocities in the range of $0.8D_{CJ} - 1.2D_{CJ}$ is used to compute a representative average detonation velocity. This criteria is based on observation from other studies, both simulations and experiments, which indicate that the detonation shock front oscillates from $0.8D_{CJ}$ to $1.2D_{CJ}$ [14, 92]. Mathematically, this averaging method is shown in Equation 5.3. The detonations observed in this study also exhibit this oscillating behavior, represented by the standard deviation bars in Figure 5.14.

$$D_{p_0} = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} (0.8D_{CJ} \ge v_{i,j} \ge 1.2D_{CJ})$$
(5.3)



Figure 5.13. Comparison of theoretical CJ calculations (CJ) and experimental measurements of detonation pressures using spark ignition (S) for C_2H_4 - N_2O and C_2H_4 - O_2 as a function of initial pressure, p_0 . Error bars indicate fluctuations in measured peak pressures.

The average detonation velocities for ethylene-O₂, shown in Figure 5.14, are higher than velocities for ethylene-N₂O, in agreement with the theoretical CJ calculations. The velocities with standard deviations for ethylene-O₂ are also higher than the CJ detonation velocities for all initial pressures considered and this is attributed to the pre-compression of the unburned mixture. However, the case with $p_0 = 20$ psia is the only initial condition for ethylene-N₂O for which the average detonation velocity with standard deviation is higher than its corresponding CJ value. For all other initial pressures greater than 20 psia, the average detonation velocities are comparable to their CJ detonation values, in spite of the pre-compression of unburned gas mixture. A possible explanation for this is that the thermal decomposition of nitrous oxide has a decreasing effect on the detonation velocity and this effect increases with initial pressure up to $p_0 = 40$ psia. Beyond this initial pressure, the mixture transitions to a detonation early in the combustion tube and the decomposition of nitrous oxide does not have a large effect on the detonation properties. However, further



Figure 5.14. Comparison of theoretical CJ calculations (CJ) and experimental measurements of detonation velocities using spark ignition (S) for $C_2H_4-N_2O$ and $C_2H_4-O_2$ as a function of initial pressure, p_0 . Error bars indicate fluctuations in measured velocities.

experiments along with a better understanding of the chemical kinetics of nitrous oxide-hydrocarbon mixtures at elevated pressures are necessary to confirm this behavior. As with the measured pressures, the velocities for ethylene-O₂ have smaller standard deviations in comparison to the nitrous oxide mixtures, with the exception of the $p_0 = 20$ psia case. Once again, this suggests a more stable detonation with oxygen as the oxidizer.

The relatively larger oscillations in the detonation pressures and velocities observed with ethylene-N₂O in comparison with ethylene-O₂ can also be explained using the detonation stability parameter χ_{Ng} developed by Ng et al. [93]. They introduced this stability parameter to characterize one-dimensional detonation stability and it is mathematically defined as:

$$\chi_{Ng} = \varepsilon_I \frac{\Delta_I}{\Delta_R} = \varepsilon_I \Delta_I \frac{\dot{\sigma}_{max}}{u_{CJ}} \tag{5.4}$$

where Δ_I and Δ_R denote the characteristic induction length and reaction length, respectively. ε_I is activation energy governing the sensitivity of the induction period, $\dot{\sigma}_{max}$ is the maximum thermicity from ZND calculations and u_{CJ} is the the particle velocity at the CJ plane in shock-fixed coordinates. Their numerical simulations of detonations in several mixtures resulted in high-amplitude, non-uniform detonation pressures and shock velocities in mixtures with high stability parameters. Based on these simulations, they defined a neutral stability criteria of $\chi_{Ng} = 1-1.5$, above which detonations have increasing levels of instability leading to irregular detonation cell structures. Additionally, Austin et al. [94] studied the reaction zone in weakly, moderately and highly unstable detonations using schlieren and PLIF imaging techniques. They observed a highly regular soot foil pattern and shock front structure for a 2H₂- O_2 -12Ar mixture with a χ_{Ng} value of 0.91, which agrees with the conclusions of Ng et al. [93]. On the contrary, the C_2H_4 - $3O_2$ - $8N_2$ mixture used by Austin et al. produced a very irregular soot foil pattern and lead shock structure. Based on calculations, they also predict that a mixture of C_3H_8 - $5O_2$ is highly unstable and this is in agreement with the stability parameter analysis in [93] ($\chi_{Ng} = 16.6$).

In accordance with this discussion on detonation stability predictions, the detonation stability parameter χ_{Ng} is calculated for ethylene-N₂O and ethylene-O₂ using the Shock and Detonation Toolbox [84] in Cantera [83]. The stability parameter χ_{Ng} increases from 20.7 to 22.1 for ethylene-N₂O and increases from 8.7 to 14.0 for ethylene-O₂ in the initial pressure range of 20 to 70 psia used in the current work. This suggests that both ethylene-N₂O and ethylene-O₂ are unstable detonations with irregular detonation cell structures. However, the relative comparison of the stability parameters for these two mixtures indicates that the detonations in ethylene-N₂O are more unstable resulting in "highly irregular" cell structures as classified in [93]. Additionally, the irregular cellular structure of the front of the accelerating deflagration in ethylene-N₂O at $p_0 = 25$ psia, shown in Figure 5.15, suggests that the subsequent detonation will be highly unstable. The flame front in the schlieren images in Figure 5.15 are 6.25 inches (2:40 ms) and 10 inches (3:30 ms) from the ignition event.



Figure 5.15. Schlieren images of the irregular cellular flame front in an ethylene-N₂O mixture at $p_0 = 25$ psia. The flame propagates in the +x direction. Flame front in the right frame is 6.25 inches (2:40 ms) from ignition and in left frame is 10 inches (3:30 ms) from ignition.

5.3.2 Ethylene Versus Acetylene (with N_2O)

Another comparison conducted in this work is between acetylene and ethylene. Acetylene is an exceptionally energetic fuel but presents serious practical storage concerns. It cannot be injected at high pressures as it is unstable above 30 psia and hence, has limited propulsion applications. A possible alternative is ethylene. Theoretical calculations for ethylene-N₂O and acetylene-N₂O indicate similar detonation properties as shown in Figures 4.1 and 4.2 of Chapter 4, which further supports the investigation of ethylene as a possible alternative to acetylene as a fuel. These two fuels are also compared using experimental measurements of the detonation properties of mixtures with nitrous oxide when ignited using spark ignition. The initial mixture pressure is varied from 20 - 70 psia in increments of 10 psia for ethylene-N₂O. However, acetylene-N₂O tests are limited to lower initial mixture pressures of 15, 18 and 20 psia, which corresponds to an operating pressure less than 30 psia on the upstream side of the metering sonic venturi on the acetylene line. This prevents explosion hazards associated with flowing acetylene above 30 psia. Ignition is achieved in all mixtures and transition to a detonation is observed at all investigated initial pressures. These average detonation pressures are plotted against initial pressure (p_0) in Figure 5.16 with the standard deviations represented by the error bars. Between the two mixtures, the measured detonation pressures are lower for acetylene-N₂O as shown in Figure 5.16. Specifically, the case with an initial pressure of 20 psia provides a direct comparison between these two mixtures where the average pressure is 14% lower for acetylene-N₂O. However, the standard deviation of peak pressures at $p_0 = 20$ psia is larger for acetylene and hence, detonation pressures for acetylene and ethylene with nitrous oxide are very comparable. As with ethylene-N₂O and ethylene-O₂, the measured detonation pressures for acetylene-N₂O at all three initial pressures are higher than the calculated CJ detonation pressures as shown in Figure 5.16 due to the pre-compression of the unburned gas mixture prior to DDT.



Figure 5.16. Comparison of theoretical CJ calculations (CJ) and experimental measurements of detonation pressures using spark ignition (S) for C_2H_4 -N₂O and C_2H_2 -N₂O as a function of initial pressure, p_0 . Error bars indicate fluctuations in measured peak pressures.

The average detonation velocities for these two mixtures are plotted against initial pressure (p_0) in Figure 5.17. The detonations observed in acetylene-N₂O also exhibit

oscillations, represented by the standard deviation bars. The predicted CJ detonation velocity curves for both ethylene-N₂O and acetylene-N₂O mixtures lie within the standard deviation of the measured velocities and these measured velocities are faster than CJ velocities for all initial pressures except at 40 and 50 psia for ethylene-N₂O and at 20 psia for acetylene-N₂O. As discussed in Section 5.3.1, this is possibly due to the thermal decomposition of nitrous oxide having a retarding effect on the detonation velocity. As with the measured detonation pressures, the average detonation velocities are also lower for acetylene-N₂O when compared to those of ethylene-N₂O. However, when taking into account the standard deviations, the detonation velocities of ethylene-N₂O mixtures appear comparable to each other.



Figure 5.17. Comparison of theoretical CJ calculations (CJ) and experimental measurements of detonation velocities using spark ignition (S) for C_2H_4 -N₂O and C_2H_2 -N₂O as a function of initial pressure, p_0 . Error bars indicate fluctuations in measured velocities.

5.3.3 Spark Ignition Versus Heated Nichrome Ignition

This work also investigates the effect of different ignition methods on the measured detonation properties of ethylene-oxidizer mixtures. A similar study was conducted by Bollinger et al. [95] where they investigated the effect of ignition methods on detonation run-up distances in hydrogen-oxygen mixtures. They used an exploding bridge wire (EBW), a nichrome glow wire and a chemical squib for ignition and reported shortest run-up distances with the chemical squib and longest with the nichrome glow wire. The authors explained that the glow wire takes a fairly long time to heat to a high temperature and the heating is also accompanied by convective heat transfer. However, both exploding bridge wire and chemical squib generated a pressure wave, with a stronger pressure wave produced by the chemical squib. In addition to the pressure wave, these two ignition methods involve fast heating and project hot particles into the gas mixture ahead of them. In comparison, the current work uses a high-voltage spark and heated nichrome wire ignition methods to ignite the combustible mixtures. The measured detonation pressures and velocities as a function of initial pressure for these two ignition methods are shown in Figures 5.18(a) and 5.18(b). It is evident from these figures that the measured pressures and velocities are very similar between the two ignition methods. The two largest differences between the ignition methods are observed for the detonation pressures of ethylene- N_2O at $p_0 = 20$ and 70 psia. The average detonation pressures with nichrome ignition are 27% ($p_0 = 20$ psia) and 14% ($p_0 = 70$ psia) higher than those measured with spark ignition. With respect to measured velocities, the largest difference is observed for ethylene-O₂ at $p_0 = 20$ psia where spark ignition produced a 3.4% higher average detonation velocity over nichrome ignition. However, Figures 5.18(a) and 5.18(b) show that even for cases with discernible differences in measured properties, the error bars overlap significantly, indicating that the measurements are in fact comparable.

This observation is explained using high-speed imaging of these two ignition processes with ethylene- N_2O in combustion tube C2 which has optical accessibility. With



Figure 5.18. Effect of ignition method on the dependence of detonation properties on initial pressure, p_0 . (S) indicates spark ignition and (N) indicates nichrome ignition. (a) Detonation pressures; (b) Detonation velocities.

spark ignition, the general process begins with high voltage (12 - 45 kV) applied to the electrodes. During the voltage rise, there is no current flow between the electrodes because the fuel-oxidizer mixture in the gap is an insulator. Once the applied voltage exceeds the dielectric strength of the gas mixture, the mixture becomes ionized. This allows a high amperage current to flow across the gap, resulting in a hot spark with temperatures on the order of a few thousand degrees K. The intense heat in the spark channel causes the ionized gas to expand very quickly, like a small explosion, producing an ignition kernel. Figure 5.19 shows the result of such an ignition process in ethylene-N₂O at $p_0 = 25$ psia where an ignition kernel is fully formed 250 μ s after the spark is actuated. In order to estimate the amount of ignition energy supplied by this method, the voltage supplied to the electrodes and the current flowing across the electrode gap are measured with the spark plug mounted in a pressure chamber. Nitrogen is used to pressurize the chamber to avoid combustion. From the current and voltage measurements, the electric breakdown between the electrodes lasts for about 20 μ s and supplies an energy between 54 - 97 mJ for the pressure range $p_0 =$ 20-70 psia. Although the combustible mixture is different from pure nitrogen, these values are a good estimate of the energy input from the spark ignition circuit.



Figure 5.19. A fully formed ignition kernel observed at the ignition plane 250 μ s after the spark ignition circuit is actuated in ethylene-N₂O at $p_0 = 25$ psia.

In comparison, the ignition event from the nichrome wire is relatively long in duration and the wire is not sufficiently hot to be captured by the high-speed camera until 9:35 ms after actuation. The nichrome heating intensifies for another 9 ms before the wire breaks and ignites the mixture. This sequence of events is shown in Figure 5.20. This process is similar to the nichrome heating description by Bollinger et al. [95] where in the process of heating the wire there is also convective heating of the mixture surrounding it. The convective heat transfer from the hot nichrome wire is captured in a sequence of high-speed schlieren images in Figure 5.21. As the nichrome heating intensifies, the wire glows red and immediately after glowing red hot breaks apart as shown in Figure 5.21(c). At this instance, the wire is close to its melting point of 1673 K and is well above the temperature at which nitrous oxide decomposes (850 K). This could initiate the unimolecular decomposition of nitrous oxide before igniting the ethylene-nitrous oxide mixture and aids in the initial combustion of the mixture leading to flame acceleration similar to that observed with spark ignition.



Figure 5.20. High-speed image sequence of (a) nichrome wire heating, (b) heated nichrome wire breaking and (c) combustible mixture ignition by heated nichrome wire. Combustible mixture is ethylene-N₂O at $p_0 = 25$ psia

However, in spite of this difference in the initial ignition process, the flame develops at a similar rate with time once the mixture is ignited. This is evident from the sequence of high-speed images, shown in Figures 5.22 and 5.23, of the accelerating flame in ethylene-nitrous oxide at $p_0 = 25$ psia ignited with a spark and heat nichrome



Figure 5.21. High-speed schlieren image sequence of convective heating of surrounding mixture caused by the hot nichrome wire.

ignition methods. Therefore, due to similar flame acceleration observed with both ignition methods, it is expected that the flame transitions to a detonation with similar properties as measured and shown in Figures 5.18(a) and 5.18(b).

5.4 Run-up Distance Measurements & Correlations

Run-up distance is defined as the distance between the source of ignition and the downstream location where the flame transitions to a detonation. As discussed in Section 5.1, to measure run-up distances with better spatial resolution, the signal from the PMT module aimed axially down the combustion tube is used. In this method, the DDT time is defined as the time from ignition to the inflection point in the PMT signal as shown in Figure 5.5. The DDT time is correlated with the pressure signals as shown in Figure 5.6 to estimate the run-up distance (L_{DDT}) . The run-up distances estimated using this method are non-dimensionalized with respect to the combustion tube diameter (d) and denoted as X_d . Figure 5.24 shows these dimensionless run-up distances on a log-log scale against initial pressure. Irrespective of the ignition method used, the run-up distances are shortest for ethylene-O₂ and longest for ethylene-N₂O, which is expected since ethylene-O₂ at $p_0 \geq 50$ psia are about 1



Figure 5.22. High-speed image sequence shows the evolution of the flame in an ethylene-N₂O mixture at $p_0 = 25$ psia ignited by spark ignition. Top image shows the ignition kernel produced by the spark ignition.

inch or shorter, indicating that the flame transitions to a detonation very close to the ignition plane. In this region, the combustion wave is either spherical or transitioning to a planar front, which increases the uncertainty of the measured run-up distances for these initial pressure cases. A similar observation was reported by Kuznetsov



Figure 5.23. High-speed image sequence shows the evolution of the flame in an ethylene-N₂O mixture at $p_0 = 25$ psia ignited by heated nichrome wire. Top image shows the ignition of the mixture right after the nichrome wire breaks apart.

et al. [17] in their measurement of run-up distances for H_2 -O₂, resulting in greater variability in the run-up distances measured for initial pressures between 1 and 8 bar (14.5 and 116.0 psi).

As shown in Figure 5.24, the dimensionless run-up distance, X_d , decreases with increasing initial pressure. To describe this pressure dependence, Nettleton suggests an inverse power law of the form [3]:

$$X_d = k p_0^{-m} \tag{5.5}$$

where, k is a constant determined empirically from experimental measurements.

Firstly, the run-up distances of fuel-oxidizer mixtures used in the current work are compared with those from other mixtures from literature. As shown in Figure 5.25, Nettleton [3] observed the power law correlation in Equation 5.5 with the run-up distance versus initial pressure measurements conducted by Bollinger et al. ([15] and [9]), where methane-O₂ produced the highest exponent of 1.25 and carbon monoxide-O₂ produced the lowest at 0.46. In comparison, the current work shows that ethylene-O₂ and ethylene-N₂O have high run-up distance dependence on initial pressure, with power law exponents of 1.52 and 1.05, respectively, for spark ignition and 1.47 and 1.42, respectively, for nichrome ignition. However, X_d for acetylene-N₂O has a weak dependence on p_0 , and similar to that of carbon monoxide-O₂. In comparison, Kuznetsov et al. [17] report a run-up distance dependence on initial pressure of $X_d = 0.7p_0^{-1.17}$ for H₂-O₂. Based on this analysis, it is evident that the run-up distance for the mixtures investigated in the current work has a very high dependence on initial pressure of the mixture. The physical and chemical processes that determine these pressure dependencies are the subject of ongoing investigation.

Another comparison of run-up distances is based on the two ignition methods used in this work. On comparing Figures 5.24(a) and 5.24(b), it is evident that the dimensionless run-up distances for a given mixture are very similar between the two ignition methods with a minor difference in its dependence on initial pressure for ethylene-N₂O. As discussed in Section 5.3.3, although a relatively long time is required to heat the nichrome wire before it ignites the mixture, the high-speed images show that the flame accelerates at a comparable rate irrespective of the ignition method. Due to this, the run-up distances are similar between the two ignition



Figure 5.24. Dimensionless detonation run-up distance (X_d) versus initial pressure (p_0) . (a) Spark ignition (S); (b) Nichrome ignition (N).



Figure 5.25. Dimensionless detonation run-up distance (X_d) versus initial pressure (p_0) measurements by Bollinger and co-workers: * [15] and [†] [9].

methods. With respect to the dependence of run-up distance on initial pressure, it is comparable with both ignition methods for ethylene- O_2 , but slightly different in the case of ethylene- N_2O . Run-up distances for ethylene- N_2O with nichrome wire ignition have a higher dependence on initial pressure than with spark ignition. This could possibly be attributed to increased decomposition of nitrous oxide due to convective heat transfer from the heating nichrome wire at higher initial pressures.

These measured run-up distances can be tested for agreement with existing flame acceleration models. As discussed in Chapter 2, one such simplified model was developed by Dorofeev [23] in which the run-up distance is estimated using Equation 2.1 and is based on theoretical flame properties and combustion tube dimensions. In his model, run-up distance is defined as the flame propagation distance where the flame speed reaches the sound speed in the combustion products. The correlation between the non-dimensional run-up distances predicted using this model and the experimental measurements is shown in Figure 5.26.



Figure 5.26. Correlation between model and experimental run-up distances based on the model developed by Dorofeev and adopted from [23]. The data set highlighted with a red box is used to verify the model.

The run-up distance data set highlighted with a red box in Figure 5.26 is from the work of Kuznetsov et al. [17] where run-up distances were measured for H₂-O₂ at $p_0 = 0.2$ - 8 bar. It should be noted that Figure 5.26 does not include all run-up distances from [17] and only includes a select data point from each initial pressure. In order to extend this analysis as part of the current work, the complete data set from [17] is used by us to independently verify this model and values for the theoretical flame properties required for the model are given in [17]. Therefore, the correlation between Dorofeevs's model and the complete set of run-up distances from [17] is shown in Figure 5.27. It is observed in this figure that the measurements do not agree well for all data points, especially at initial pressures greater than 1 bar. On reviewing the theoretical flame properties for H₂-O₂ in the range of $p_0 = 0.2$ - 8 bar and from Equation 2.1, Dorofeev's model has a strong dependence on the laminar flame speed (S_L) of the mixture. For H₂-O₂ the laminar flame speed increases from 7.1 m/s for $p_0 = 0.2$ bar to 10.2 m/s for $p_0 = 0.8$ bar, but asymptotes for higher initial pressures. Additionally, other flame properties used in the model do not vary in this range of initial pressures, which leads to the disagreement of model predictions with run-up distance measurements in mixtures with weak or no dependence of the laminar flame speed on initial pressure. A similar disagreement is observed between Dorofeev's model and measurements from the current work with ethylene-oxidizer mixtures as shown in Figure 5.28. Acetylene-N₂O measurements are not included in this analysis as the range of initial pressures for this mixture is very small and does not provide any additional insight on the performance of the model for varying pressures. As shown in Figure 4.7(a), the laminar flame speed remains approximately constant for ethylene-N₂O and increases by only 0.9 m/s for ethylene-O₂ in the range of initial pressures investigated. In addition to this, the other flame properties also remain approximately constant with initial pressure. Therefore, Dorofeev's model cannot predict the strong dependence of the run-up distance on pressure observed in this work. Therefore, any model that would apply across large pressure ranges would need to capture the effect of pressure on the flame acceleration and/or detonation properties, and Dorofeev's model does not.



Figure 5.27. Correlation between Dorofeev's model [23] and experimental run-up distances measured by [17].



Figure 5.28. Correlation between Dorofeev's model [23] and experimental run-up distances measured in the current work for ethyleneoxidizer mixtures.

Another model which aims to correlate detonation run-up distance with flame properties was developed by Bollinger et al. [15] and is discussed in detail Chapter 4. They derived an empirical function called the K function, defined in Equation 4.3, to correlate with measured run-up distances. Values of K are calculated for the mixtures and initial pressures from the current work and are plotted against the measured nondimensional run-up distances in Figure 5.29 along with the measurements by Bollinger et al. [15, 96]. As discussed by the authors of [15], the methane-O₂ system does not exhibit a unique relationship with the K function unlike the non-hydrocarbon systems. However, the ethylene-O₂ results from this work somewhat agree with the correlation formed by the H₂-O₂ and CO-O₂ systems. The results from ethylene-N₂O do not follow this relationship but coincide with the correlation for methane-O₂ mixture with methane mole percent less than 50%.

Finally, the run-up distances measured in the current work are correlated with the ZND exothermic pulse widths calculated using the Shock and Detonation Toolbox



Figure 5.29. Dimensionless run-up distance vs. correlation function K for various mixtures from current work and from Bollinger et al.: [†] [96], [‡] [15].

[84] and are shown in Figure 5.30. In addition to measurements from the current work, two other run-up distance data sets from literature are used for comparison: measurements by Kuznetsov et al. [17] for H_2 -O₂ and by Li et al. [18] for propane-O₂. These two data sets are chosen for comparison as they use a method and criteria to quantify run-up distance similar to that used in the current work. As shown in Figure 5.30, there is a good correlation between the non-dimensional run-up distance and the ZND exothermic pulse width for these mixtures. This suggests that there may exist a universal correlation between the non-dimensional run-up distance of a mixture and its calculated ZND exothermic pulse width which can be used to estimate run-distances for mixtures and initial conditions without actually measuring it.

5.5 Deflagrations & Pre-compression in Nitrous Oxide Mixtures

As discussed in the Section 5.3.1 and shown in Figure 5.13, the measured detonation pressures are higher than the CJ values for all initial pressures and mixtures



Figure 5.30. Correlation between non-dimensional run-up distance and ZND exothermic pulse width for mixtures from the current work and two other mixtures from $[17](\dagger)$ and $[18](\ddagger)$

tested. This discrepancy is due to the phenomenon of pre-compression or "pressure piling" of the unburned gas mixture ahead of the combustion wave. Pre-compression or pressure piling arises during the deflagration stage when the flame acts like a piston and compresses the combustible mixture ahead of it. Therefore, DDT occurs in a mixture with higher initial pressure, resulting in a measured detonation pressure much greater than the theoretical CJ value without pre-compression [3]. Coincidentally, as the initial pressure of combustible mixture increases, there is a noticeable decrease in the average over-pressure factor, indicating a lower degree of pre-compression of the combustible mixture due to faster DDT (shorter run-up distance). At lower initial pressures flame transition to detonation is slower leading to larger pre-compression.

5.5.1 Pre-compression Factors and Direct Measurement

According to CJ theory, there is a linear correlation between CJ detonation pressure and initial pressure as shown in Figure 4.2(a). Therefore, by measuring the detonation overpressure in these tests, the new initial pressure (that is, the precompression pressure) of the detonation is estimated by using the same linear relationship. Based on this, a pre-compression factor denoted by δ is defined as the ratio of the average detonation pressure (P_{p_0}) to CJ detonation pressure or

$$\delta = \frac{P_{p_0}}{P_{CJ}} = \frac{\frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} (p_{i,j} \ge P_{CJ})}{P_{CJ}}$$
(5.6)

where, $p_{i,j}$ is the peak pressure from i^{th} test and j^{th} pressure transducer location.

Table 5.2 lists the pre-compression factors estimated using Eq. 5.6 for all mixtures and initial pressures investigated in this study. The pre-compression factors follow the same relative order as the measured pressures, with ethylene-N₂O resulting in the highest factors and ethylene-O₂ the lowest. This relative order is also illustrated in Table 5.2 with a one-to-one comparison of pre-compression factors for all mixtures at $p_0 = 20$ psia. A consequence of the higher pre-compression with ethylene versus acetylene is the higher average detonation pressures for ethylene-N₂O over acetylene-N₂O as shown in Figure 5.16. Additionally, the reported pre-compression of the unburned gas mixture results in increased CJ values, which are compatible with the measured detonation velocities and pressures.

In addition to determining pre-compression factors for these mixtures based on dynamic pressure measurements, two piezoresistive pressure transducers from Kulite[®] are used as described in Section 5.1.5 to directly measure the pressure of compression waves produced by the accelerating flame. These measurements are conducted for ethylene-N₂O at $p_0 = 20$ and 30 psia only since the flame accelerates over a longer section of the combustion tube and the pressure from the compression waves can be measured for a longer time duration. An example of the pressure signals produced by these compression waves as a function of time is shown in Figure 5.7. The increasing

Initial Pressure, p_0 [psia]	$\mathbf{C}_{2}\mathbf{H}_{4} extsf{-}\mathbf{N}_{2}\mathbf{O}$ (Spark)	$\mathbf{C}_{2}\mathbf{H}_{4}\text{-}\mathbf{O}_{2}$ (Spark)	$\mathbf{C}_{2}\mathbf{H}_{2} extsf{-}\mathbf{N}_{2}\mathbf{O}$ (Spark)	$\mathbf{C}_{2}\mathbf{H}_{4}\text{-}\mathbf{N}_{2}\mathbf{O}$ (Nichrome)	$\mathbf{C}_{2}\mathbf{H}_{4}\text{-}\mathbf{O}_{2}$ (Nichrome)
15	-	3.19	2.94	-	-
18	-	-	2.73	-	-
20	3.03	2.39	2.59	3.85	2.51
30	2.59	2.10	-	2.87	2.09
40	2.41	2.02	-	2.70	2.02
50	2.34	1.84	-	2.36	1.88
60	2.23	1.66	-	2.31	1.79
70	1.93	1.51	-	2.19	1.72

Table 5.2. Pre-compression factors at different initial pressures for mixtures in this study.

pressure in Figure 5.7 is indicative of the progressively stronger compression waves produced by the deflagration due to its acceleration. As time progresses and the deflagration accelerates to higher velocities, it coalesces with the compression waves and eventually transitions to a detonation. As described in Section 5.1.5, the times at which discrete compression waves reach the two Kulite[®] sensors could be used to estimate the distance-time path of the accelerating flame based on 1D unsteady gas dynamics. The following sub-section describes the theory and resulting flame path estimates.

5.5.2 1D Unsteady Gas Dynamics Model of Flame Acceleration

The flow field encountered in the propagation of explosive waves and detonations is typically unsteady flow. So, one-dimensional unsteady gas dynamics can be used to describe the flow physics observed in the current work. The flow associated with detonations is typically 2D or highly 3D, so using this 1D approximation is a simplified model but can be easily applied analytically and used to help interpret the data. The gas dynamics model is a concise version of the mathematical analysis described in *Gas Dynamics* by Zucrow and Hoffman [97] and can be referred to for more details. For simplicity, the 1D model assumes homentropic flow (constant entropy) of a compressible fluid, in the absence of work and body forces. An unsteady homentropic flow is a flow for which the entropy remains constant throughout the flow field for all time. Based on the assumptions, the governing equations for unsteady 1D homentropic flow are:

Continuity equation:
$$\frac{d\rho}{dt} + \nabla .(\rho \mathbf{V}) = 0$$
 (5.7)

Momentum equation:
$$\rho \frac{D\mathbf{V}}{dt} + \nabla p = 0$$
 (5.8)

Energy equation:
$$\rho \frac{D}{Dt} \left(h + \frac{V^2}{2} \right) - \frac{dp}{dt} = 0$$
 (5.9)

Entropy equation:
$$\frac{Ds}{Dt} = 0$$
 (5.10)

Since the flow is assumed homentropic, the speed of sound definition may be employed in place of the energy equation:

$$\frac{Dp}{Dt} - a^2 \frac{D\rho}{Dt} = 0 \tag{5.11}$$

The continuity and speed of sound equations are combined and expressed in one spatial dimension in Equation 5.12 and the momentum equation in cartesian form is shown in Equation 5.13.

$$\rho a^2 \frac{\partial u}{\partial x} + \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} = 0$$
(5.12)

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial p}{\partial x} = 0$$
(5.13)

For a homentropic flow, the density ρ is a unique function of the pressure p throughout the flow and thus

$$\rho = \rho(p). \tag{5.14}$$

The characteristic and compatibility equations corresponding to Equations 5.12 and 5.13 are determined by multiplying these equations by the unknown parameters σ_1 and σ_2 , respectively, and summing:

$$\sigma_1(5.12) + \sigma_2(5.13) = 0. \tag{5.15}$$

The characteristic curves are the paths in space and time along which information is propagated through a flow field and the compatibility equation is the ordinary differential equation derived by combining the partial differential conservation equations. For this, u(x,t) and p(x,t) are assumed to be continuous functions so that

$$\frac{du}{dx} = \frac{\partial u}{\partial x} + \lambda \frac{\partial u}{\partial t} \quad \text{and} \quad \frac{dp}{dx} = \frac{\partial p}{\partial x} + \lambda \frac{\partial p}{\partial t}.$$
(5.16)

where $\lambda = dt/dx$ or the slope of the characteristics. Expanding and rearranging Equation 5.15 and combining with Equation 5.16 yields the compatibility equation for 1D unsteady homentropic flow

$$(\rho u\sigma_1 + \rho a^2\sigma_2)du + (\sigma_1 + u\sigma_2)dp = 0$$
(5.17)

and the characteristic equations for this flow are

$$\lambda = \frac{\sigma_1}{u\sigma_1 + a^2\sigma_2} = \frac{\sigma_2}{\sigma_1 + u\sigma_2}.$$
(5.18)

Finally, eliminating the unknown parameters σ_1 and σ_2 from Equations 5.17 and 5.18 and solving for the slope of the characteristics λ yields

$$\lambda_{\pm} = \left(\frac{dt}{dx}\right)_{\pm} = \frac{1}{u \pm a}.$$
(5.19)

From every point on the space-time or x - t plane of an unsteady flow, there exist two characteristics C_+ and C_- corresponding to the + and - signs, respectively, in Equation 5.19. Hence, Equation 5.19 states that the propagation speed along C_{\pm} characteristics is equal to the speed of sound relative to the moving fluid. In that regard, the C_{\pm} characteristics in unsteady flow are analogous to the Mach lines in a steady supersonic flow. Assuming the gas experiences an isentropic process, the compatibility equation can be further simplified by combining with the ideal gas equation and $a^2 = \gamma RT = \gamma p/\rho$ to yield

$$a_{\pm}^* \pm \frac{\gamma - 1}{2} u_{\pm}^* = constant \tag{5.20}$$

where $a^* = a/a_0$, $u^* = u/a_0$ and a_0 is the speed of sound in some initial undisturbed portion of the flow. Then, the flow properties T, p and ρ corresponding to the value of a^* are determined using the isentropic relations:

$$p_{\pm}^* = (T_{\pm}^*)^{\gamma/(\gamma-1)} = (a_{\pm}^*)^{2\gamma/(\gamma-1)}$$
(5.21)

$$\rho_{\pm}^* = (a_{\pm}^*)^{2/(\gamma-1)} \tag{5.22}$$

where $p^* = p/p_0$, $T^* = T/T_0$ and $\rho^* = \rho/\rho_0$.

This 1D unsteady homentropic flow model can be used as a simplified model for the accelerating deflagration prior to DDT. Such an accelerating deflagration from the current work is schematically illustrated in Figure 5.31, where the deflagration is represented by a piston accelerating from left to right. The flame accelerates from rest at time t = 0 into a stationary gas (u = 0). The initial motion of the flame produces a small pressure disturbance that propagates to the right into the undisturbed fluid with the speed of sound a. Hence, the velocity of the front of the wave is $(dx/dt)_{+} = a$, because a right-running wave is a C_{+} characteristic.

The wave created by the initial piston motion imparts a pressure increment dp > 0and a velocity increment du > 0 to the initially undisturbed gas, and is, therefore, a compression wave. For an isentropic process, if dp > 0 then da > 0. As the piston continues to accelerate, successive compression waves are generated at the face of the piston and move into the disturbed gas. The latter has a velocity, u,



Figure 5.31. Schematic representation of the deflagration as an accelerating piston producing compression waves.



Figure 5.32. Estimation of flame path for Test 362, constructed using temporal pressure measurements of compression waves produced by the accelerating deflagration. Estimation is based on 1D unsteady homentropic flow analysis.

and speed of sound, a, larger than the corresponding values for the undisturbed gas. Consequently, the speeds of propagation, $(dx/dt)_+ = u + a$, of the consecutive waves increase, and each wave travels faster than the preceding wave. The slopes of the C_+ characteristics, given by $(dt/dx)_+ = 1/(u+a)$, become more and more horizontal and the waves converge, as illustrated in Figure 5.32.

A typical piston or flame path, is indicated in Figure 5.32. Typically in such problems the flame or piston path is known which is used to estimate the 1D flow field in the unburned gas mixture. However, in the current work, pressure measurement as a function of time in two adjacent locations is known, as shown in Figure 5.7. So, this information is used to estimate the flame or piston path in the combustion tube. If we consider the ignition plane at x = 0, the two pressure transducers are installed at $x_{k1} = 4.378$ inches (11.12 cm) and $x_{k2} = 10.378$ (26.36 cm) from the ignition plane. From Figure 5.7, the times of arrival of a compression wave of pressure p_i at these two locations are extracted and their (x, t) coordinates are plotted on the spacetime plane. A line connecting these two points forms one of the C_+ characteristics on Figure 5.32 as flow properties do not change along a characteristic curve. The slope of this C_+ characteristic yields the speed of sound relative to the moving fluid. Using this information, the velocity of the flame U_{fL_i} and coordinates (x_{p_i}, t_{p_i}) are determined following the algorithm in Figure 5.33. This process is iterated with a dppressure increment until the combustion wave arrives at the first pressure transducer location. Once the flame velocity profile is estimated, the flame path is determined starting from x = 0 and $t = t_{ign}$. In spite of the assumptions made in this model, it provides a good estimate for the flame path and closely coincides with the time and

provides a good estimate for the flame path and closely coincides with the time and location of the first PCB transducer measurement as shown in Figure 5.32 for Test 362 and this is true for all five tests in this series.

The estimated flame paths and corresponding velocities from this analysis for all five tests in this series are shown in Figures 5.34(a) and 5.35(a), respectively. The estimated velocity profile as a function of time has an exponential trend for all tests and an example of this trend for Test 361 is shown in Figure 5.35(a). The preexponential factors and exponents on all these exponential trends are different from each other and depend on the initial flame development. This trend is in accordance with the theory proposed by Liberman et al. [21] and represented by Equation 4.2. The initial pressures chosen for these tests are only slightly different from each other and so the estimated flame velocities are similar for the five cases.



Figure 5.33. Flowchart explaining the method to estimate the flame path of an accelerating deflagration using pressure measurements. Method is based on 1D unsteady homentropic flow analysis.

These 1D estimates are qualitatively compared to the flame path measured from high-speed imagining of the accelerating flame in combustion tube C2. Three tests are conducted to directly image the flame, two with spark ignition and one with heated nichrome wire, in a mixture of ethylene-N₂O at $p_0 = 25$ psia. Although this initial pressure is in the range of initial pressures investigated in combustion tube C1, the flame acceleration observed in the two tubes are slightly different from each other. In combustion tube C1, the unburned gas mixture is confined by an unbreakable metal end wall, whereas a diaphragm is used to maintain the initial pressure in combustion tube C2 which ruptures as soon as the compression waves from the accelerating



Figure 5.34. Flame path on space-time plane. (a) Estimates based on 1D unsteady flow analysis for the five tests conducted in this series.; (b) Measurements from high-speed imaging. Inset: comparison between direct tracking of flame and 1D estimate



Figure 5.35. Flame velocity as a function of time. (a) Estimates based on 1D unsteady flow analysis. The trendline associated with the velocity profile of Test 361 is shown for reference.; (b) Measurements from high-speed imaging.

flame coalesce and reflect from it. Due to rupturing of the diaphragm, some of the unburned gas mixture feeding the propagating flame is exhausted from the tube, thereby reducing flame acceleration and preventing DDT. This is a consequence of the shorter length of combustion tube C2 in comparison to tube C1 which is longer by a factor of 2.5. The rupturing of the diaphragm at the end of tube C2 is shown in a sequence of high-speed schlieren images in Figure 5.36 for a mixture of ethylene- N_2O at $p_0 = 25$ psia. The left frame in the figure shows the coalescing of incident compression waves on the diaphragm, the middle frame shows a compression wave reflected from the diaphragm and the right frame shows the diaphragm rupturing leading to the exhaust of unburned gases. In spite of this difference between the two combustion tubes, the flame path estimated from the 1D analysis can be qualitatively compared with that measured from high-speed images. These high-speed images are captured at a rate of 20 kHz and the observed flame propagation is shown in Figures 5.22 and 5.23 with spark and heated nichrome ignition, respectively.



Figure 5.36. Rupturing of diaphragm on combustion tube C2, before the flame arrives at the exit, due to reflection of compression waves produced by the accelerating flame. Middle and right frames are captured 100 and 150 μ s after the left frame. Left: coalescing of incident waves on diaphragm; Middle: reflected wave moving along -x; Right: rupture of diaphragm due to reflected pressure.

The experimentally measured flame path and velocity profiles for all three tests at $p_0 = 25$ psia in combustion tube C2 are shown in Figures 5.34(b) and 5.35(b), respec-

tively. On comparing Figures 5.34(a) and 5.34(b), the flame path estimated by the 1D model based on pressure measurements of the compression waves is different from that measured from high-speed imaging. As discussed in the previous paragraph, this is attributed to the different lengths of the two combustion tubes and confinements of the unburned gas mixture. The inset in Figure 5.34(b) shows a direct comparison between an example flame path estimated by the 1D model and an example of that measured from high-speed imaging. The comparison shows that both flame paths are non-linear with time, but have different degrees of non-linearity. This difference is also reflected in the velocity profiles from 1D analysis in comparison to those measured using high-speed imaging. The 1D estimates yield an exponential dependence of flame velocity on time, but the high-speed images show an approximately linear dependence of the velocity on time. In addition to the differences in the two combustion tubes used for these tests, another, more important difference between these two flame paths is that the flame tracked by high-speed imaging is 2D or 3D whereas the estimated flame path is based on 1D analysis. The 1D unsteady model is a simplified approximation of an accelerating flame which is far from being one-dimensional and can only provide a close estimate of the flame path.

Finally, the high-speed schlieren imaging system is used to capture compression waves produced by the accelerating flame in combustion tube C2. A sequence of schlieren images in Figure 5.37 shows one such compression wave propagating in the +x direction. The velocity of this compression wave is determined by knowing the imaging frame rate and the displacement of the wave. Based on this information, the compression wave is moving at a velocity of 315.6 m/s in the +x direction. For reference, the speed of sound in a mixture of ethylene-N₂O at the initial room temperature is 279.0 m/s. This implies that the compression wave is propagating in an pre-compressed or pre-heated gas mixture at 397 K which has a higher sound speed. Using this information in the isentropic pressure ratio relation, Equation 5.21, yields a pressure ratio of 3.19 across the compression wave. In comparison, pre-compression factors estimated for ethylene-N₂O with spark ignition in Table 5.2 are 3.03 and 2.59
for initial pressures of 20 and 30 psia, respectively. The pressure ratio of the compression wave captured by imaging is slightly higher, but similar to the estimates in Table 5.2 which suggests that the method used to estimate these pre-compression factors is a reasonable assessment of the pre-compression caused by the accelerating flame.



Figure 5.37. Schlieren image sequence of a compression wave produced by the accelerating flame in an ethylene-N₂O mixture at $p_0 = 25$ psia. The field of view is located between 20.75 and 22.75 inches from the ignition plane. The compression wave propagates in the +x direction. Middle and left frames are captured 50 and 100 μ s after the right frame.

6. SUMMARY

In this work, the detonation, DDT and deflagration characteristics of ethylene-nitrous oxide are investigated experimentally and theoretically in comparison with other traditional bipropellant mixtures at initial pressures above 1 atm. For this purpose, two combustion tubes are designed and fabricated in-house. One of the combustion tubes (C1) has circular cross-section and is developed to study detonation properties and is completely fabricated out of steel. The other combustion tube (C2) has a rectangular cross-section and is developed to provide optically access to the accelerating flame with full-length polycarbonate sheets on two sides and a rupture diaphragm for pressure relief from the combustion wave. Three fuel-oxidizer mixtures, ethylene- N_2O , ethylene- O_2 and acetylene- N_2O , are studied experimentally when ignited with spark ignition or heated nichrome wire ignition. The experiments characterize the performance of ethylene-N₂O and compare it with that of ethylene-O₂, which is a more traditional mixture. Additionally, detonation properties of ethylene-N₂O are compared with those of acetylene- N_2O to present ethylene as an alternative fuel to the more energetic but unstable acetylene. The use of two ignition methods provides an insight into the effect of different ignition methods on the measured detonation properties. The three mixtures always produce detonation pressures in excess of CJ values. The measured velocities are comparable to CJ velocity calculations for the two nitrous oxide mixtures, but are higher for ethylene- O_2 .

The detonation characteristics of ethylene- N_2O are first compared with those of ethylene- O_2 to assess the relative performance of these two oxidizers. The nitrous oxide mixture produces higher detonation pressures and lower detonation velocities in comparison to the oxygen mixture, which is consistent with Chapman-Jouget detonation calculations. However, the standard deviations of the measured pressures and velocities suggest that, in general, nitrous oxide mixtures produce higher oscillations in detonation properties as the detonation propagates along the combustion tube. This is likely due to the monopropellant nature of nitrous oxide, which exothermically decomposes at elevated temperatures. With increasing initial pressure, we believe that this thermal decomposition of nitrous oxide also has a decreasing effect on the measured detonation velocities, resulting in velocities comparable to calculated CJ values in spite of the pre-compression of unburned mixture. The relatively large detonation pressure and velocity oscillations observed in ethylene-N₂O mixtures is also explained using the detonation stability parameter χ_{Ng} developed by Ng et al. [93]. Although both ethylene-oxidizer mixtures have stability parameters well above the neutral stability criteria, the parameter for ethylene-N₂O ($\chi_{Ng} = 21.4$) is about twice as high as that for ethylene-O₂ ($\chi_{Ng} = 11.3$) and indicates highly unstable detonations in nitrous oxide mixtures. This explains the large pressure oscillations observed with ethylene-N₂O.

The detonation measurements from this work also show that $ethylene-N_2O$ produces higher average detonation pressures and velocities in comparison to acetylene- N_2O , which is contrary to CJ calculations. This discrepancy can be explained by the higher pre-compression level observed in ethylene-N₂O mixtures prior to DDT, resulting in higher starting pressures in the combustible mixture ahead of the combustion wave. Therefore, the resulting detonation pressures are higher for this mixture. The lower pre-compression level in acetylene- N_2O is due to shorter run-up distances, allowing less time for pre-compression of the unburned gas mixture. Hence, the choice of fuel between ethylene and acetylene depends on the application requirement of whether faster DDT or higher detonation pressure is desired. However, when accounting for the range of the pressure oscillations, the detonation properties of these two mixtures are comparable and the run-up distance dependence on initial pressure for acetylene- N_2O is weaker than that exhibited by ethylene- N_2O . This suggests that for ethylene- N_2O , some mechanism that is promoting DDT is becoming stronger at higher initial pressures, resulting in faster DDT. All these factors support ethylene as a viable fuel alternative to acetylene.

The measured detonation properties resulting from these two ignition methods are very similar. The two largest differences are observed between the detonation pressures of ethylene-N₂O at $p_0 = 20$ and 70 psia where the average detonation pressures with nichrome ignition are 27% and 14%, respectively, higher than that measured with spark ignition. However, the significant overlap of standard deviations for these cases indicate that the measurements are comparable. High-speed imagining of the two ignition processes show that the high-voltage spark produces an ignition kernel immediately after the ignition circuit is actuated which develops into an accelerating flame soon after. The spark is caused by the electric breakdown of the discharge gap between the electrodes and this produces high temperatures and free radicals which accelerate the process of mixture ignition. In comparison, the ignition event from the nichrome wire is much slower, as a relatively long time is required before the wire is hot enough to break apart and ignite the mixture. At this instance, the wire is close to its melting point of 1673 K and is well above the temperature at which nitrous oxide decomposes (850 K). This could initiate the unimolecular decomposition of nitrous oxide before igniting the ethylene-nitrous oxide mixture and aids in the initial combustion of the mixture leading to flame acceleration similar to that seen with spark ignition.

In addition to detonation pressure and velocity, the run-up distance at which deflagration-to-detonation transition occurs is also quantified by the measuring the light emitted by the combustion wave using a PMT module installed axially on the combustion tube. Ethylene- O_2 mixtures exhibit shorter run-up distances compared to ethylene- N_2O with both ignition methods and therefore higher pre-compression of the unburned mixture is achieved with ethylene- N_2O . As suggested by Nettleton [3], the run-up distances non-dimensionalized with tube diameter for the three mixtures follow an inverse power law dependence with initial pressure, similar to other measurements by Bollinger et al. [9, 15]. However, these run-up distance measurements do not correlate with the model developed by Dorofeev [23] as the analytical expression for the run-up distance relationship has a strong dependence on laminar flame speed of

the mixture. The laminar flame speeds of the mixtures investigated in the current work remain approximately constant with initial pressure and so the measured run-up distances disagree with Dorofeev's model. Therefore, Dorofeev's model cannot predict the strong dependence of the run-up distance on pressure observed in this work. Therefore, any model that would apply across large pressure ranges would need to capture the effect of pressure on the flame acceleration and/or detonation properties, and Dorofeev's model does not. The run-up distances exhibit some correlation with the empirical K function developed by Bollinger et al. [15]. The results from the ethylene- O_2 system follow the trendline associated with the H_2 - O_2 and CO- O_2 and those from the ethylene- N_2O system agree with the trend of stoichiometric and lean CH_4 - O_2 data points. Additionally, the run-up distance measurements correlate well with the calculated ZND exothermic pulse width for all three mixtures from the current work and for two other data sets from literature which use a method of runup distance quantification similar to that used in the current work. This suggests that there may exist a universal correlation between the non-dimensional run-up distance of a mixture and its calculated ZND exothermic pulse width which can be used to estimate run-distances for mixtures and initial conditions without actually measuring it.

The pre-compression of the unburned gas mixture caused by the accelerating flame prior to DDT is estimated as the ratio of average detonation pressure to CJ detonation pressure. The pre-compression factors are highest for ethylene-N₂O and lowest for ethylene-O₂. The pre-compression is also measured directly using two piezoresistive pressure transducers for two initial pressures. These pre-compression measurements are used in a 1D unsteady homentropic gas dynamics model to estimate the path followed by the accelerating deflagration. In spite of the assumptions made in this model, it provides a good estimate for the flame path and closely coincides with the time and location of the first PCB transducer measurement for all tests in this series. A direct comparison between the flame path estimated by the 1D model in combustion tube C1 and that measured from high-speed imaging in combustion tube C2 shows that both flame paths are non-linear with time, but have different degrees of non-linearity. This difference is also reflected in the velocity profiles from 1D analysis in comparison to those measured using high-speed imaging. The 1D estimates yield an exponential dependence of flame velocity on time, but the high-speed images show an approximately linear dependence of the velocity on time. An important reason for this difference between these two flame paths is that the flame tracked by high-speed imaging is 2D or 3D whereas the estimated flame path is based on 1D analysis. The 1D unsteady model is a simplified approximation of an accelerating flame which is far from being one-dimensional and can only provide a close estimate of the flame path.

The high-speed schlieren imaging system is also used to capture the compression waves produced by the accelerating flame in tube C2. One of the compression waves propagates at a velocity of 315.6 m/s, which is significantly higher than the speed of sound in the initial mixture. This indicates that the wave is propagating into an unburned mixture that is already pre-heated or pre-compressed from earlier, weaker compression waves. Using the propagation velocity of this compression wave along with isentropic relations yields a pressure ratio of 3.19 across the compression wave. In comparison, pre-compression factors estimated for ethylene-N₂O with spark ignition are 3.03 and 2.59 for initial pressures of 20 and 30 psia, respectively. The pressure ratio of the compression wave captured by imaging is slightly higher, but similar to the pre-compression factors is a reasonable assessment of the pre-compression caused by the accelerating flame.

7. RECOMMENDATIONS

This work included the study of detonations and DDT in a combustion tube of L/d= 68 (C1). From the tests conducted in C1, it is evident that the flame transitions to a detonation within the first half of the tube for most initial conditions investigated. The additional length of the tube ensures that the compression waves reflected from the closed end of the tube do not interact with the accelerating deflagration. In comparison, combustion tube C2 is less than half the length of C1 and high-speed schlieren images of the deflagration captures the interaction of the flame and reflected waves. Since C2 is not equipped to measure steep-fronted pressure waves, modifying the design of C1 ensures the study of detonations resulting from such a flame reflected wave interaction. This investigation could benefit the gas handling industry as compression waves produced by accidental flames in pipelines could reflect from bends or closed sections and interact with the flame in delivery lines. Altering C1 such that it is constructed as multiple sections with flanges permits measurements in varied lengths of closed tube. Additionally, these sections can be made short enough to allow honing of the inner surface to have better control on the surface finish as roughness of the combustion tube is proven to influence the phenomenon of DDT.

The comparison between the two ignition methods used in this work result in similar detonation properties, but exhibit some differences in the initial flame development. The convective heating associated with the heated nichrome wire ignition method could initiate nitrous oxide decomposition as opposed to the direct reaction between fuel and nitrous oxide. This difference in reaction paths for the two ignition methods is another area which requires further investigation.

Two existing analytical models used to correlate measured run-up distances with flame properties are used to understand the complex dependence of DDT on theoretical parameters. There is a weak agreement of the results from the current work to one of the models, but fails with the other. However, the measured run-up distances from this work and two other data sets formed a general trend with the ZND exothermic pulse width of the mixtures. Future work includes the development of a general correlation between run-up distance and parameter which is a combination of calculated flame and ZND properties and/or reaction rates of dominant elementary reactions. Additional flame or DDT visualization tests at different initial pressures in C2 could benefit this investigation as well. The combustion tube C2 can be extended in length to ensure the flame transitions to a detonation. This can be achieved by attaching a flange to the open end of C2 which in interfaces with a extension section. Similar investigations done by Kuznetsov et al. [17] use a rectangular channel of 50 \times 50 mm cross section and 3.4 m long and capture the DDT event.

A few recommendations are made to improve on the preliminary study conducted to investigate the dependence of pressure transducer installation configuration on pressure measurement. In this study, all four PCB pressure transducers are installed in the same plane similar to earlier tests conducted on this setup. Due to this, it is possible that one port could have an influence on the pressure measured by a pressure transducer in an adjacent or opposite port. This argument is based on some unpublished preliminary simulations performed by another researcher which requires further investigation. Another possible factor that could influence the measurements in a recess cavity is the use of different combustible mixtures. If the amplification measured by a pressure transducer mounted in a recess cavity port shown in Appendix B is caused by constant volume combustion in the cavity or due to the reactive reflective wave, then the combustion regime and properties in the cavity are different depending on the combustible mixture used for the study. This could be due to difference in cell widths or combustion limits in correlation to the 5-mm diameter of the recess. Based on the preliminary measurements to investigate this effect, these additional effects are highlighted for further investigation to fully explain the phenomenon causing this effect. In combination with these analyses, the development of a transfer function to correlate pressure measurement in a recess cavity port to that in a flush port form a separate study on its own.

REFERENCES

- [1] E. Mallard and H. Le Chatelier. *Recherches expérimentales et théoriques sur la combustion des mélanges gazeux explosives.* H. Dunod et E. Pinat, 1883.
- [2] J H S Lee. *The Detonation Phenomenon*, volume 2. Cambridge University Press Cambridge, 2008.
- [3] M A Nettleton. Gaseous Detonations: their nature, effects and control. Springer Science & Business Media, 2012.
- [4] D L Chapman. On the rate of explosion in gases. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 47(284):90–104, 1899.
- [5] E Jouguet. Sur la propagation des réactions chimiques dans les gaz. Journal de Mathématiques Pures et Appliquées, 1:347–425, 1905.
- [6] P Bangalore Venkatesh, J D'Entremont, S E Meyer, S P M Bane, and M C Grubelich. High-pressure combustion and deflagration-to-detonation transition in ethylene/nitrous oxide mixtures. In 8th U.S. National Combustion Meeting, 2013.
- [7] J A Laughrey, L E Bollinger, and R Edse. Detonability of nitrous oxide at elevated initial temperature and pressure. Technical report, ARL 62-432: Aerospace Research Laboratories, 1962.
- [8] U Pfahl, E Schultz, and J E Shepherd. Detonation cell width measurements for H₂-N₂O-N₂-O₂-CH₄-NH₃ mixtures. Technical report, FM98-5: Explosion Dynamics Laboratory, 1998.
- [9] L E Bollinger, J A Laughrey, and R Edse. Experimental detonation velocities and induction distances in hydrogen-nitrous oxide mixtures. ARS Journal, 32:81–82, January 1962.
- [10] R Akbar and J Shepherd. Detonations in N₂O-H₂-N₂-air mixtures. Technical report, Prepared for Los Alamos National Laboratory Under Consultant Agreement C-4836, 1993.
- [11] R Akbar, M J Kaneshige, E Schultz, and J E Shepherd. Detonations in H₂-N₂O-CH₄-NH₃-O₂-N₂ mixtures. Technical report, FM97-3: Explosion Dynamics Laboratory, 1997.
- [12] M Kaneshige, E Schultz, U J Pfahl, J E Shepherd, and R Akbar. Detonations in mixtures containing nitrous oxide. In Proceedings of the 22nd International Symposium on Shock Waves, Imperial College, London, UK, volume 1, pages 251–256, 2000.

- [13] R Mével, F Lafosse, L Catoire, N Chaumeix, G Dupré, and C E Paillard. Induction delay times and detonation cell size prediction of hydrogen-nitrous oxidediluent mixtures. *Combustion Science and Technology*, 180(10-11):1858–1875, 2008.
- [14] R Mével, D Davidenko, F Lafosse, N Chaumeix, G Dupré, C E Paillard, and J E Shepherd. Detonation in hydrogen-nitrous oxide-diluent mixtures: An experimental and numerical study. *Combustion and Flame*, 162(5):1638-1649, 2015.
- [15] L E Bollinger, M C Fong, and R Edse. Experimental measurements and theoretical analysis of detonation induction distances. ARS Journal, 31(5):588–595, 1961.
- [16] M Wu, M P Burke, S F Son, and R A Yetter. Flame acceleration and the transition to detonation of stoichiometric ethylene/oxygen in microscale tubes. *Proceedings of the Combustion Institute*, 31(2):2429–2436, 2007.
- [17] M Kuznetsov, V Alekseev, I Matsukov, and S B Dorofeev. DDT in a smooth tube filled with a hydrogen–oxygen mixture. *Shock Waves*, 14(3):205–215, 2005.
- [18] J Li, W H Lai, K Chung, and F K Lu. Uncertainty analysis of deflagration-todetonation run-up distance. *Shock Waves*, 14(5-6):413–420, 2005.
- [19] B L Wang, M Habermann, M Lenartz, H Olivier, and H Grönig. Detonation formation in H₂-O₂/He/Ar mixtures at elevated initial pressures. *Journal of Shock Waves*, 10(4):295–300, September 2000.
- [20] C S Wen, K M Chung, Y C Hsu, and F K Lu. Smoked foil on deflagration-todetonation transition. *Journal of Propulsion and Power*, 31(3):967–970, May– June 2015.
- [21] M A Liberman, M F Ivanov, A D Kiverin, M S Kuznetsov, A A Chukalovsky, and T V Rakhimova. Deflagration-to-detonation transition in highly reactive combustible mixtures. Acta Astronautica, 67(7):688–701, 2010.
- [22] V Bychkov, A Petchenko, V Akkerman, and L E Eriksson. Theory and modeling of accelerating flames in tubes. *Journal of Physical Review E*, 72(4):046307, 2005.
- [23] S B Dorofeev. Hydrogen flames in tubes: Critical run-up distances. International Journal of Hydrogen Energy, 34(14):5832–5837, 2009.
- [24] M F Ivanov, A D Kiverin, I S Yakovenko, and M A Liberman. Hydrogen–oxygen flame acceleration and deflagration-to-detonation transition in three-dimensional rectangular channels with no-slip walls. *International Journal of Hydrogen En*ergy, 38(36):16427–16440, 2013.
- [25] J Vandooren, M C Branch, and P J Van Tiggelen. Comparisons of the structure of stoichiometric CH₄-N₂O-Ar and CH₄-O₂-Ar flames by molecular beam sampling and mass spectrometric analysis. *Combustion and Flame*, 90(3-4):247–258, 1992.
- [26] O A Powell, P Papas, and C Dreyer. Laminar burning velocities for hydrogen-, methane-, acetylene-, and propane-nitrous oxide flames. *Combustion Science* and *Technology*, 181(7):917–936, 2009.

- [27] C J Rallis, A M Garforth, and J A Steinz. Laminar burning velocity of acetyleneair mixtures by the constant volume method: Dependence on mixture composition, pressure and temperature. *Combustion and Flame*, 9(4):345–356, 1965.
- [28] G Von Elbe and M Mentser. Further studies of the structure and stability of burner flames. The Journal of Chemical Physics, 13(2):89–100, 1945.
- [29] W G Parker and H G Wolfhard. Some characteristics of flames supported by NO and NO₂. In *International Symposium on Combustion*, volume 4(1), pages 420–428. Elsevier, 1953.
- [30] O A Powell, P Papas, and C B Dreyer. Hydrogen- and C_1-C_3 hydrocarbonnitrous oxide kinetics in freely propagating and burner-stabilized flames, shock tubes, and flow reactors. *Combustion Science and Technology*, 182(3):252–283, 2010.
- [31] M T Allen, R A Yetter, and F L Dryer. Hydrogen/nitrous oxide kineticsimplications of the N_xH_y species. Combustion and Flame, 112(3):302–311, 1998.
- [32] S P M Bane, R Mével, S A Coronel, and J E Shepherd. Flame burning speeds and combustion characteristics of undiluted and nitrogen-diluted hydrogen-nitrous oxide mixtures. *International Journal of Hydrogen Energy*, 36(16):10107–10116, 2011.
- [33] R Mével, F Lafosse, N Chaumeix, G Dupré, and C E Paillard. Spherical expanding flames in H₂-N₂O-Ar mixtures: flame speed measurements and kinetic modeling. *International Journal of Hydrogen Energy*, 34(21):9007–9018, 2009.
- [34] S Coronel, R Mével, S P M Bane, and J E Shepherd. Experimental study of minimum ignition energy of lean H₂-N₂O mixtures. *Proceedings of the Combustion Institute*, 34(1):895–902, 2013.
- [35] E L Litchfield. Minimum ignition-energy concept and its application to safety engineering. Technical report, Bureau of Mines, Pittsburgh, PA (USA), 1959.
- [36] H Henrici and S H Bauer. Kinetics of the nitrous oxide-hydrogen reaction. The Journal of Chemical Physics, 50(3):1333–1342, 1969.
- [37] W Jost, K W Michel, J Troe, and H G Wagner. Untersuchung des thermischen zerfalls von N₂O in stoßwellen. Zeitschrift für Naturforschung A, 19(1):59–64, 1964.
- [38] R I Soloukhin. High-temperature oxidation of hydrogen by nitrous oxide in shock waves. In *International Symposium on Combustion*, volume 14(1), pages 77–82. Elsevier, 1973.
- [39] R I Soloukhin and P J Van Tiggelen. Shock tube study of the induction lag in nitrous oxide-hydrogen system. Bulletin des Sociétés Chimiques Belges, 78(3-4):179–189, 1969.
- [40] A Duval and P J Van Tiggelen. Kinetical study of hydrogen-nitrous oxide flames (kinetics of flames propagating in hydrogen-nitrous oxide mixtures diluted with inert gases). Academie Royale de Belgique, Classe des Sciences, Bulletin, 53(4):366-402, 1967.

- [42] R Mével, S Javoy, F Lafosse, N Chaumeix, G Dupré, and C E Paillard. Hydrogennitrous oxide delay times: Shock tube experimental study and kinetic modelling. *Proceedings of the Combustion Institute*, 32(1):359–366, 2009.
- [43] J M Hall, S Reehal, and E L Petersen. Kinetics of OH chemiluminescence in the presence of silicon. *Chemical Physics Letters*, 425(4):229–233, 2006.
- [44] S Pichon. Etude cinétique de systèmes hypergoliques et propergoliques à base d'éthanol et de peroxyde d'hydrogène. PhD thesis, Orléans, 2005.
- [45] R Mével, S Pichon, L Catoire, N Chaumeix, C E Paillard, and J E Shepherd. Dynamics of excited hydroxyl radicals in hydrogen-based mixtures behind reflected shock waves. *Proceedings of the Combustion Institute*, 34(1):677–684, 2013.
- [46] S Zabarnick. A comparison of CH₄/NO/O₂ and CH₄/N₂O flames by LIF diagnostics and chemical kinetic modeling. *Combustion Science and Technology*, 83(1-3):115–134, 1992.
- [47] D J Seery and C T Bowman. An experimental and analytical study of methane oxidation behind shock waves. *Combustion and Flame*, 14(1):37–47, 1970.
- [48] Y Hidaka, H Takuma, and M Suga. Shock-tube studies of N₂O decomposition and N₂O-H₂ reaction. Bulletin of the Chemical Society of Japan, 58(10):2911– 2916, 1985.
- [49] M T Allen, R A Yetter, and F L Dryer. The decomposition of nitrous oxide at $1.5 \le P \le 10.5 atm$ and $1103 \le T \le 1173K$. International Journal of Chemical Kinetics, 27(9):883–909, 1995.
- [50] M Röhrig, E L Petersen, D F Davidson, and R K Hanson. The pressure dependence of the thermal decomposition of N₂O. International Journal of Chemical Kinetics, 28(8):599–608, 1996.
- [51] S Javoy, R Mével, and C E Paillard. A study of N_2O decomposition rate constant at high temperature: Application to the reduction of nitrous oxide by hydrogen. International Journal of Chemical Kinetics, 41(5):357–375, 2009.
- [52] M C Grubelich, D King, S Knudsen, D Blankenship, S Bane, and P Venkatesh. An overview of a high energy stimulation technique for geothermal applications. In World Geothermal Congress, 31070, pages 19–25, Melbourne, Australia, April 2015. International Geothermal Association.
- [53] P Bangalore Venkatesh, J H D'Entremont, S E Meyer, S P M Bane, M C Grubelich, and D K King. Bipropellant high energy stimulation for oil and gas applications. Journal of Petroleum Science and Engineering, 180:660–667, 2019.
- [54] P Bangalore Venkatesh, T Graziano, S P Bane, S Meyer, and M C Grubelich. Deflagration-to-detonation transition in nitrous oxide-ethylene mixtures and its application to pulsed propulsion systems. In 55th AIAA Aerospace Sciences Meeting, page 0372, 2017.

- [55] P Bangalore Venkatesh, S E Meyer, S P M Bane, and M C Grubelich. Deflagration-to-detonation transition in nitrous oxide/oxygen-fuel mixtures for propulsion. *Journal of Propulsion and Power*, 35(5):1–9, 2019.
- [56] Z Krilov, B Kavedzija, and T Bukovac. Advanced well stimulation method applying a propellant based technology. *Drilling*, *Oil*, *Gas*, 25(2):405–416, 2008.
- [57] R W Humble, G N Henry, and W J Larson. Space propulsion analysis and design. McGraw-Hill, 1995.
- [58] M J Tauschek, L C Corrington, and M C Huppert. Nitrous oxide supercharging of an aircraft engine cylinder. NACA Wartime Report E-199, National Advisory Committee for Aeronautics. Lewis Flight Propulsion Lab, Cleveland, OH, United States, June 1945.
- [59] A Jost, K W Michel, J Troe, and H G Wagner. Detonation and shock-tube studies of hydrazine and nitrous oxide. Technical report, Aerospace Research Laboratories Report ARL 63-157, Wright-Patterson Air Force Base, 1963.
- [60] C Merrill. Nitrous oxide explosive hazards. Technical report, Air Force Research Laboratory Technical paper, AFRL-RZ-ED-TP-2008-184, 2008.
- [61] Airgas (Air Liquide). Nitrous oxide explosion. Technical report, U.S. Chemical Safety and Hazard Investigation Board, Report Number: 2016-04-I-FL, 2017.
- [62] M C Grubelich, J Rowland, and L Reese. A hybrid rocket engine design for simple low cost sounding rocket use. In *Joint Propulsion Conference and Exhibit*, volume 1, 1993.
- [63] J S Tyll and R Herdy. The nitrous oxide-propane rocket engine. Technical report, GASL TR No. 387: Micro Craft Inc., Huntsville, AL, 2001.
- [64] R DiSalvo, M Ostrander, and A Elliott. Constant volume rocket motor, 2009. US Patent 7,631,487.
- [65] J Foust. The space review: Essays and commentary about the final frontier. Technical report, http://www.thespacereview.com/article/2543/1, June 2014.
- [66] L Werling, N Perakis, S Müller, A Hauck, H Ciezki, and S Schlechtriem. Hot firing of a N₂O/C₂H₄ premixed green propellant: First combustion tests and results. In Space Propulsion Conference, 2016.
- [67] B Zhang, H D Ng, R Mével, and J H S Lee. Critical energy for direct initiation of spherical detonations in H₂/N₂O/ar mixtures. *International Journal of Hydrogen Energy*, 36(9):5707–5716, May 2011.
- [68] A Karabeyoglu, J Dyer, J Stevens, and B Cantwell. Modeling of N₂O decomposition events. In 44th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, AIAA 2008-4933, Hartford, CT, July 2008.
- [69] M Kuznetsov, J Grune, and S Jallais. Decomposition of N₂O. dynamics of explosion and flame propagation. In *European Combustion Meeting 2017*, Dubrovnik, Croatia, April 2017.

- [70] B Zhang, H D Ng, and J H S Lee. The critical tube diameter and critical energy for direct initiation of detonation in C₂H₂/N₂O/ar mixtures. *Combustion and Flame*, 159(9):2944–2953, September 2012.
- [71] C J Brown and G O Thomas. Experimental studies of shock-induced ignition and transition to detonation in ethylene and propane mixtures. *Combustion and Flame*, 117(4):861–870, June 1999.
- [72] B Varatharajan and F A Williams. Ethylene ignition and detonation chemistry, part 1: Detailed modeling and experimental comparison. *Journal of Propulsion* and Power, 18(2):344–351, March-April 2002.
- [73] K Kailasanath. Recent developments in the research on pulse detonation engines. AIAA journal, 41(2):145–159, February 2003.
- [74] M Kuznetsov, M Liberman, and I Matsukov. Experimental study of the preheat zone formation and deflagration to detonation transition. *Combustion Science and Technology*, 182(11-12):1628–1644, October 2010.
- [75] M-H Wu and T-H Lu. Development of a chemical microthruster based on pulsed detonation. Journal of Micromechanics and Microengineering, 22(10):105040, September 2012.
- [76] J Li, P Zhang, L Yuan, Z Pan, and Y Zhu. Flame propagation and detonation initiation distance of ethylene/oxygen in narrow gap. Applied Thermal Engineering, 110:1274–1282, January 2017.
- [77] R P Lindstedt and H J Michels. Deflagration to detonation transitions and strong deflagrations in alkane and alkene air mixtures. *Combustion and Flame*, 76(2):169–181, May 1989.
- [78] R Knystautas, J H Lee, and C M Guirao. The critical tube diameter for detonation failure in hydrocarbon-air mixtures. *Combustion and Flame*, 48:63–83, 1982.
- [79] J Li, W H Lai, K Chung, and F K Lu. Experimental study on transmission of an overdriven detonation wave from propane/oxygen to propane/air. *Combustion* and Flame, 154(3):331–345, August 2008.
- [80] J D'Entremont, R M Gejji, P Bangalore Venkatesh, and S P Bane. Plasma control of combustion instability in a lean direct injection gas turbine combustor. In 52nd Aerospace Sciences Meeting, page 0622, 2014.
- [81] P A Urtiew and A K Oppenheim. Experimental observations of the transition to detonation in an explosive gas. *Proceedings of the Royal Society of London A*, 295(1440):13–28, November 1966.
- [82] M J Bedard. Detailed Measurement of ORSC Main Chamber Injector Dynamics. PhD thesis, School of Aeronautics & Astronautics, Purdue University, West Lafayette, Indiana, USA, 2017.
- [83] D Goodwin. Cantera: Object-oriented software for reacting flows. Technical report, California Institute for Technology (Caltech): www.code.google.com/p/cantera, 2005.

- [84] S Browne, J E Shepherd, and J L Ziegler. Shock and Detonation Toolbox. Technical report, California Institute for Technology (Caltech): www2.galcit.caltech.edu/EDL/public/cantera/html/SD_Toolbox/index.html, 2005.
- [85] S Kao and J E Shepherd. Numerical solution methods for control volume explosions and ZND detonation structure. Technical report, FM-2006: Galcit Report, 2008.
- [86] I A Zeldovich, G I Barenblatt, V B Librovich, and G M Makhviladze. Mathematical Theory of Combustion and Explosions. Consultants Bureau, New York, NY, 1985.
- [87] K K Kuo. *Principles of Combustion*. Wiley New York et al., 1986.
- [88] A D Craven and T R Greig. The development of detonation over-pressures in pipelines. In *Institution of Chemical Engineering Symposium Series*, volume 25, pages 41–50, 1968.
- [89] G Thomas, G Oakley, and R Bambrey. An experimental study of flame acceleration and deflagration to detonation transition in representative process piping. *Journal of Process Safety and Environmental Protection*, 88(2):75–90, March 2010.
- [90] C B Kiyanda, V Tanguay, A J Higgins, and J H S Lee. Effect of transient gasdynamic processes on the impulse of pulse detonation engines. *Journal of Propulsion and Power*, 18(5):1124–1126, September 2002.
- [91] J Fischer, C Liebner, H Hieronymus, and E Klemm. Maximum safe diameters of microcapillaries for a stoichiometric ethene/oxygen mixture. *Chemical Engineering Science*, 64(12):2951–2956, June 2009.
- [92] J E Shepherd. Detonation in gases. Proceedings of the Combustion Institute, 32(1):83–98, 2009.
- [93] H D Ng, M I Radulescu, A J Higgins, N Nikiforakis, and J H S Lee. Numerical investigation of the instability for one-dimensional chapman–jouguet detonations with chain-branching kinetics. *Combustion Theory and Modelling*, 9(3):385–401, 2005.
- [94] J M Austin, F Pintgen, and J E Shepherd. Reaction zones in highly unstable detonations. Proceedings of the Combustion Institute, 30(2):1849–1857, 2005.
- [95] L E Bollinger, R Edse, and J A Laughrey. Effect of ignition method on detonation induction distances in hydrogen-oxygen mixtures. ARS Journal, 32(3):428–430, 1962.
- [96] L E Bollinger, R Edse, M C Fong, and J A Laughrey. Experimental and theoretical studies on the formation of detonation waves in variable geometry tubes. Technical report, D-1983: Prepared for NASA Under Grant NsG-44-60 by Ohio State University, 1963.
- [97] M J Zucrow and J D Hoffman. Gas Dynamics, Vol. I. John Wiley & Sons Inc, New York City, 1976.

[98] K S Schwinn, B Kan, S V Sardeshmukh, R M Gejji, S D Heister, and C D Slabaugh. Self-excited, multi-khz dynamics in a linear, semi-bounded detonation channel. In 55th AIAA Aerospace Sciences Meeting, page 0375, 2017.

A. PRESSURE AND VELOCITY PLOTS

A.1 Spark Ignition, Ethylene-Nitrous Oxide







A.2 Spark Ignition, Ethylene-Oxygen







A.3 Spark Ignition, Acetylene-Nitrous Oxide





A.4 Heated Nichrome Ignition, Ethylene-Nitrous Oxide







A.5 Heated Nichrome Ignition, Ethylene-Oxygen









B. A STUDY ON THE DEPENDENCE OF PRESSURE TRANSDUCER INSTALLATION CONFIGURATION ON DETONATION PRESSURE MEASUREMENT

As mentioned in Chapter 5, a consequence of installing high-frequency pressure transducers in a recess port to measure steep-fronted pressure waves is the attenuation/amplification and phase distortion of the measured pressure signal. So, its characterization in the presence of a steep-fronted high pressure wave encountered in detonation studies is important, but has not been conducted carefully. In order to characterize the effect of pressure transducer installation on the measurement of steep fronted waves, a preliminary study is conducted and a modular experimental setup is designed and installed at Maurice J. Zucrow Labs.

The steep-fronted detonation wave is generated using an existing hydrogen-oxygen pre-detonator which is used to initiate combustion in a linear Rotating Detonation Wave Combustor (RDWC) experiment [98]. The pre-detonator is fed by independently controlled supplies of hydrogen and oxygen with separate sonic venturis on each propellant line to set required mass flow rates. This test setup is designed with a hexagonal stainless steel block which accommodates four PCB 109C11 pressure transducers, two flush and two recess mounted, in the same plane. A 60-inch long, 0.5-inch outer diameter stainless steel tube is connected between the pre-detonator and the hexagonal block to ensure sufficient length over which the hydrogen-oxygen combustion wave transitions to a fully developed planar detonation. On the downstream of the pressure transducer plane, there is a vent valve to exhaust combustion products, a low-frequency pressure transducer and thermocouple to monitor initial conditions of the combustible mixture and a fixed venturi VACCON Min J Series vacuum ejector to evacuate the combustion chamber prior to propellant fill. The effective inner diameter of this combustion tube is 0.402 inches and this dimension is much larger than the cell width of hydrogen-oxygen mixtures at 14.7 psia or above. A schematic of this experimental setup is shown in Figure B.1 and a cross-sectional view of the pressure transducer plane with details of both the installation configurations is shown in Figure B.2. This setup is an improvement over its predecessor used for a similar study using PCB 113B26 and Kulite WCT-312M-35BARA pressure transducers and provides more control over the initial conditions of the combustible mixture in the tube. The flush configuration ensures that the sensing element of the pressure transducer is flush with the inner surface of the combustion chamber, while the recessed configuration is a replication of the configuration used in the pressure transducer ports on combustion tube C1 (Figure 5.3).



Figure B.1. Schematic of the pressure transducer installation calibration setup for PCB 109C11 transducers.

In the pressure transducer calibration test setup, steep-fronted pressure waves are measured for five initial pressures in the range of 14.6 - 69.0 psia. This produces a wide range of detonation pressures which aids in developing a correlation between pressures measured by flush and recess mounted pressure transducers. An example of the pressure-time history measured by the four PCB pressure transducers is shown in Figure B.3 for a stoichiometric hydrogen-oxygen mixture at 14.6 psia. Figure B.3 shows two main differences between the flush and recessed pressure signals a time-lag of 6.6 μ s and an amplification of the recessed pressure amplitudes over



Figure B.2. Cross-sectional view of section A-A from Figure B.1 showing the pressure transducer plane having two flush and two recess cavity installations of PCB 109C11 transducers with recess cavity details.

the flush pressure amplitudes by 248%. The average time-lag between the flush and recessed pressure signals reduces from 6.6 μ s to 4.4 μ s with an increase in initial pressure from 14.6 psia to 69.0 psia due to an increase in detonation velocity with increasing initial pressure. The pressure signals are used to produce two correlations: measured flush peak pressures versus calculated CJ detonation pressures using Shock and Detonation Toolbox (SDT) and measured flush peak pressures versus measured recess peak pressures. The first correlation is shown in Figure B.4 and is important to understand that the measured detonation pressures are higher than the predicted CJ detonation pressures post-DDT due to the phenomenon of pre-compression of unburned gases by the accelerating flame prior to DDT. It is also important to note from Figure B.4 that the measured steep fronted pressures vary more as the initial pressure is increased. The second correlation is shown in Figure B.5 is a preliminary step in the process to correct peak pressures measured in a recess cavity based on flush mounted pressure transducers.



Figure B.3. Pressure signals from a stoichiometric hydrogen-oxygen mixture at $p_0 = 14.6$ psia.



Figure B.4. Correlation between flush mounted pressure and calculated CJ detonation pressure for stoichiometric hydrogen-oxygen.

This preliminary series of tests is not sufficient to explain the phenomenon causing the difference in measured pressures between flush and recess mounted pressure transducers shown in Figure B.5. Due to this, a correction based on this work is not yet applied to the pressure measurements in the nitrous oxide detonation work presented in this document. The measurements from the preliminary tests conclude



Figure B.5. Correlation between flush mounted and recess mounted pressures for stoichiometric hydrogen-oxygen.

two properties of the recess cavity design used for PCB pressure transducers in this work. Firstly, the steep-fronted pressure wave is amplified by the recess cavity of the pressure transducer port, which is contrary to the typical attenuation expected from a recess cavity port. Secondly, the flush mounted transducers measure pressures higher than CJ pressures (1.3 - 2.7 times CJ pressures) and this is evidence of pre-compression in the unburned gas mixture caused by the accelerating flame thereby producing detonations with elevated properties than predicted by CJ theory. Based on these preliminary tests, a few recommendations are discussed in Chapter 7 which could help fully explain the effect of pressure transducer installation configuration on pressure measurement.

C. TEST PROCEDURES

This appendix contains the test operating procedures for the operation of the Closed Tube Detonation Test Stand, also dubbed the "Sandia Fracking Test Setup", in the courtyard of the High Pressure Laboratory at Zucrow Labs. Some aspects of the highfrequency data acquisition system have changed over the years and any student using this setup to run detonation experiments must coordinate with the current staff and students to familiarize themselves with the latest procedures to record high-frequency data.
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Purdue University West Lafayette, IN



High Pressure Lab Fracking Test Operating Procedures (Longer Tube)

Test Date: Test Conductor: Project Engineer: Additional Test Operators:

Prepared by: Jonathan Chrzanowski/Heather Wiest Updated by: Prashanth Bangalore

Updated: 25-Sep-2014

Printed: 1-Nov-2017 at 19:27

A. Preliminary Setup

1. Initial Safety and Startup

_		Completed	Comments
_	Control Room:		
_	Complete TOR		
_	Record ambient pressure and temperature on TOR		
_	Verify absence of lightning within 20 miles of Test Facility		
_	Courtyard and Rocket Cell:		
_	Verify test article & igniter are installed correctly		
_	Verify Nitrogen Purge Needle Valve NV-N2-901 is Fully OPEN		
_	Verify accuracy of appropriate patching with instrumentation list		
_	Power on Main Data/Control System and any additional auxiliary data system computers		
_	Set up and power on appropriate video cameras and audio system		
_	Main Data/Control System Computer (Laptop):		
_	Record Main Data/Control System Computer IP Address (Laptop IP Address)		
_	Connect the NI USB cord to the laptop and verify laptop is connected to power outlet		
_	Start Fracking Test main data/control VI		
_	Set appropriate scan list and display list		
_	Connect the Instrumentation Power cord to the power outlet		
_	Verify all actuated valves in default/de-energized position		
_	Connect the Valve Power cord to a separate power outlet extension near the calibration panel		
_	Turn on Valve Power on the control box		
_	High Speed Data Acquisition System:		
1	Power off Data System, if necessary, before connecting any instrumentation		
_	Connect BNC cables on the electrical box to the Data System (Use slots 1 to 10 behind the system)		
_	Connect PCB cables to the electrical box and roll cable bundle to the PCB transducers		
1	Ensure appropriate ICP cards are installed on the Data System and power ON the system		
1	Connect Yellow BNC cables (1 to 10) to cards on the front panel of Data System (use only 0 to 3 CHs on each card) and circuit is completed.		
_	Remote login to Data System using: bazinga.ecn.purdue.edu; Username: Test Operator; Password:		

#@HFDAQ@!		
Launch data acquisition VI: HF_DAQ(LV2013-TimedAuto) \rightarrow HFDAQ_main.vi		
Initialization Tab: Activate necessary Cards (Dev) and Channels (CH)		
Set necessary scan rate and hit "Initialize all settings"		
DAQ Tab: Load "Channel Label" names		
Select "View TDMS file"		
2. Nitrogen Actuated Valve Operation System Set-Up		
	Completed	Comments
Coordinate N ₂ System status with Rocket, Container, Gas Turbine, and Annex test operations. If inactive, complete the following:		
LOX Room Panel:		
Verify 1500 psi Pilot Pressure Valve MV-N2-11 closed		
Verify 1500 psi Pilot Pressure Regulator MR-N2-04 is unloaded		
Verify 100 psi Pilot Pressure Valve MV-N2-10 closed		
Verify 100 psi Pilot Pressure Regulator, MR-N2-03 is unloaded		
Verify Fuel Trickle Purge Isolation Valve MV-N2-07 closed		
Unload Fuel Trickle Purge Regulator MR-N2-02 (if necessary)		
Verify Oxidizer Trickle Purge Isolation Valve MV-N2-08 closed		
Unload Oxidizer Trickle Purge Regulator MR-N2-01		
Verify Cell C Trickle Purge Isolation Valve MV-N2-204 closed		
Unload Cell C Trickle Purge Regulator MR-N2-204		
Verify Drying Station Isolation valve is closed		
Verify Drying Station Regulator MR-N2-05 is unloaded		
Verify Calibration Panel Isolation Valve MV-300 closed		
N2 Tube Trailers:		
Verify N2 Primary Tube Trailer Pressure greater than 2000 psi		
Verify Primary Tube Trailer Station Vent Valve MV-N2-05 closed		
Verify Primary Tube Trailer Station Valve PV-N2-02 open		
Verify Primary Tube Trailer 1-inch Isolation Valve MV-N2-04 open		
Verify Primary Tube Trailer Bypass Valve MV-N2-06 closed		
2		

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Fracking Test Operating Procedures (Long Tube)

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Verify Pilot Pressure Source Valve MV-N2-09 open		
Slowly open all three primary tube trailer isolation valves		
LOX Room Panel:		
Open Oxidizer Trickle Purge Isolation Valve MV-N2-08		
Load Oxidizer Trickle Purge Regulator MR-N2-01 to ~20 psig		
Open Fuel Trickle Purge Isolation Valve MV-N2-07		
	Completed	Comments
Load Fuel Trickle Purge Regulator MR-N2-02 to ~20 psig		
Open Cell C Trickle Purge Isolation Valve MV-N2-204 (if necessary)		
Load Cell C Nitrogen Trickle Purge Regulator MR-N2-204 to ~10 psig (if necessary)		
Open Pilot Pressure Source Valve MV-N2-10		
Load 100 psi Pilot Pressure Regulator MR-N2-03 to 100 psig		
Verify Nitrous Oxide Cylinder Valve MV-OX-901 is Closed		
Verify Nitrous Oxide Pressure Regulator MR-OX-901 is Unloaded		
Verify Fuel Cylinder Valve MV-FU-901 is Closed		
Verify Fuel Pressure Regulator MR-FU-901 is Unloaded		
Test Cell SCAB Regulator Panel:		
Verify Nitrogen Purge Regulator MR-N2-901 is Unloaded		
Open Nitrogen Isolation Valve MV-N2-70		

B. Valve Checks

		Completed	Comments
Courtyard/Control Room (Main Da	ta/Control System Computer):		
Turn rocket cell access safety lights to yellow			
Announce valve checks to all nearby personnel			
Cycle Nitrous Oxide Tank Valve PV-OX-901	[Closed]		
Cycle Bulk Nitrogen System Valve PV-N2-901	[Closed]		
Cycle Ethylene Tank Valve PV-FU-901	[Closed]		
Cycle Vent Valve PV-N2-902	[Closed]		
Cycle Vent Valve PV-N2-903	[Closed]		

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C. Acquisition of Zero Data

	Comp	leted	Comments
Main Data/Control System Computer:			
Open Vent Valve PV-N2-902			
Open Vent Valve PV-N2-903			
Open Nitrous Oxide Isolation Valve PV-OX-901			
Open Fuel Isolation Valve PV-FU-901			
Verify accurate pressure transducer readings			
Verify accuracy of any additional installed instrumentation			
Adjust PT and TC intercept values as required on the VI to read ambient values as per TOR			
Close Nitrous Oxide Isolation Valve PV-OX-901			
Close Fuel Isolation Valve PV-FU-901			
Close Vent Valve PV-N2-902			
Close Vent Valve PV-N2-903			

D. Final Set-Up and Safety Checks

1. Set Nitrous Oxide Pressure Regulator and Clear Test Cell

	Completed	Comments
Verify Rocket Cell, Gas Turbine Cell and Courtyard is free of persons and debris		
Load Nitrogen Purge Regulator MR-N2-901 to the desired pressure per the TOR		
	Completed	Comments
Verify Nitrous Oxide Needle Valve NV-OX-901 is fully OPEN		
Open Nitrous Oxide Bottle Valve MV-OX-901		
Load Nitrous Oxide Pressure Regulator MR-OX-901 to the desired pressure per the TOR		

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2. <u>Place necessary Chains and Set Fuel Pressure Regulator</u>

Compreted	Comments
Completed	Comments

3. Prepare for Testing

	Com	pleted		Comments	_
Set Rocket Cell, Gas Turbine Cell and LOX Room access safety lights to RED					
Set Traffic Light to RED					

4. Load Timing

	Com	oleted	Comments
Load Digital Output Timing on the VI as Per TOR			

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E. Fracking Combustion Tests

	Completed	Comments
Control System Computer:		
Verify accurate pressure transducer readings		
Verify scan rate set per TOR		
Set file details and record main data file details on TOR		
Toggle "Acquire Data" on the main VI		
Toggle "Prepare Acquire Data" on the high frequency data VI		
Record high frequency data names on TOR		
Verify Nitrogen Purge Valve PV-N2-901 is closed		
Verify Vent Valve PV-N2-902 is open		
Verify Vent Valve PV-N2-903 is open		
	Completed	Comments
Open Nitrous Oxide Isolation Valve PV-OX-901 to purge the reactor vessel		
After 30 seconds Close PV-N2-903 and monitor PT-N2-901 to rise to 20 psia		
When PT-N2-901 reaches 20 psia close PV-OX-901		
Allow PT-N2-901 to stabilize		
Open PV-N2-903 to vent reactor vessel to atmosphere		
Close PV-N2-903		
Close PV-N2-902		
Initialize video recording		
Start auto sequence		
Initiate high speed data acquisition at correct time per test auto sequence		
Terminate recording of high speed data		
Test complete		
Stop video recording		
Wait 2 minutes and open Vent Valve PV-N2-902		
Open Nitrogen Purge Valve PV-N2-901 for two minutes to purge out combustion products		
Close Nitrogen Purge Valve PV-N2-901		
Set Rocket Cell and Gas Turbine Cell access safety lights YELLOW		

Review acquired test data				
Inspect status/condition of the reactor vessel and test setup				r
Repeat sections D and E as required per test results and the Fracking Test Matrix				
F. When All Tests Completed: Venting and Reactor Purge				1
	Completed	I	Comments	_
Close Nitrous Oxide Bottle Valve MV-OX-901				-
Close Fuel Bottle Valve MV-FU-901				
Open Vent Valve PV-N2-903				
Open Vent Valve PV-N2-902				
Open Nitrogen Purge Valve PV-N2-901				_
Open Nitrous Oxide Isolation Valve PV-OX-901 for 30 sec to vent the Oxidizer from the system				-
Close Nitrous Oxide Isolation Valve PV-OX-901				
Unload Nitrous Oxide Pressure Regulator MR-OX-901				-
Open Fuel Isolation Valve PV-FU-901 for 30 sec to vent the Fuel from the system				
Close Fuel Isolation Valve PV-FU-901				
Unload Fuel Pressure Regulator MR-FU-901				-
Close Nitrogen Purge Valve PV-N2-901				-
Close Vent Valve PV-N2-902				
Close Vent Valve PV-N2-903				-
Close Nitrogen Isolation Valve MV-N2-70				
IInload Nitrooen Duroe Valve MR-N2-901				

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G. Securing Test Cell from Test Operations

	Compl	eted	Comments
Turn all access safety lights to Green			
Turn traffic light to Green			
Data System Enclosure:			
Turn off valve power on the control box and disconnect the power cord			
Turn off instrumentation power by disconnecting the power cord			
Shut down all data acquisition systems			
	Compl	eted	Comments
Power down and put away audio/video equipment			
Clean up test area			
Coordinate N2 system status with Rocket, Gas Turbine, and Annex test operations. If system shut-down required, complete the following:			
LOX Room:			
Verify 1500 psi Pilot Pressure Valve MV-N2-10 closed			
Close 100 psi Pilot Pressure Valve MV-N2-11			
Unload 100 psi Pilot Pressure Regulator MR-N2-03			
Verify 1500 psi Pilot Pressure Regulator MR-N2-04 unloaded			
Tube Trailers:			
Close all primary tube trailer isolation valves			
Open Primary Tube Trailer 1-inch Isolation Valve MV-N2-04			
Slowly open Primary Tube Trailer Vent Valve MV-N2-05 to vent system			
When system is vented close Primary Tube Trailer Vent Valve MV-N2-05			
Close Primary Tube Trailer 1-inch Isolation Valve MV-N2-04			
LOX Room Panel:			
Verify Oxidizer Trickle Purge Isolation Valve MV-N2-08 is Open			
Load Oxidizer Trickle Purge Regulator MR-N2-01 to ~20 psig			
Verify Fuel Trickle Purge Isolation Valve MV-N2-07 is Open			
Load Fuel Trickle Purge Regulator MR-N2-02 to ~20 psig			
Verify Cell C Trickle Purge Isolation Valve MV-N2-04 is Open (if necessary)			

Load Cell C Nitrogen Trickle Purge Regulator MR-N2-04 to ~10 psig (if necessary)		
I. Emergency Procedures		
Pressurized Vessel and control to Main Laptop is lost:	Completed	Comments
Disconnect Valve Power from the power outlet near the Calibration Panel		
Try and re-connect with the Main Laptop		
If unable to re-connect, ensure gases have stopped venting from the vessel using the audio system		
Return to the courtyard and unload Nitrous Oxide regulator MR-OX-901 and close the bottle valve MV-OX-901		
Unload Fuel regulator MR-FU-901 and close the bottle valve MV-FU-901		
Check the main laptop for issues and reboot the VI on the main laptop		
Bring back valve power and try remote connecting to the laptop again and ensure valves are cycling		
Damaged/Disassembled Test Setup	Completed	Comments
If valve are still active, ensure Nitrous Oxide and Fuel Isolation Valves PV-OX-901 and PV-FU-901 are closed		
Open Nitrogen Purge Valve PV-N2-901 for 30 sec to vent reactants/combustion gases		
Close Nitrogen Purge Valve PV-N2-901		
Ensure there are no flames visible on the video		
Disconnect Valve Power from the power outlet near the Calibration Panel		
Return to the courtyard and unload Nitrous Oxide regulator MR-OX-901 and close the bottle valve MV-OX-901		
Unload Fuel regulator MR-FU-901 and close the bottle valve MV-FU-901		
Inspect the damage on the test setup and assess what went wrong		
Unauthorized personnel in the testing areas	Completed	Comments
Use Mic in the control room and announce that a test is running and they should leave test area immediately		

D. ENGINEERING DRAWINGS

This appendix contains engineering drawings of all parts used to construct both combustion tubes C1 and C2. The are referred to in Chapter 3 while discussing the construction of the tubes.







Figure D.2. Engineering drawing of the propellant delivery end block for tube C1.





























VITA

Prashanth Bangalore Venkatesh

RESEARCH INTERESTS

Deflagration-to-Detonation Transition and flame acceleration; Detonation engines; Combustion; Chemical propulsion; Propellant performance characterization; Heat transfer; Experimental design and validation.

EDUCATION

- Ph.D. in Aeronautical and Astronautical Engineering, Purdue University, West Lafayette, IN, USA, 2019. Thesis: "A Study of Detonations, DDT and Deflagrations in High Pressure Ethylene-Nitrous Oxide Mixtures". Advisor: Sally P. M. Bane. GPA: 4.0/4.0
- M.S. in Aeronautical and Astronautical Engineering, Purdue University, West Lafayette, IN, USA, 2015. Advisor: Sally P. M. Bane. GPA: 3.95/4.0.
- B.E. in Mechanical Engineering, R V College of Engineering, Bangalore, India, May 2011. Thesis: "Flow Analysis of Intake Duct using NUMECA Software". Advisor: Vimala Narayanan (GTRE) & Prasad C. S. GPA: 9.46/10.0

TECHNICAL SKILLS

Experimental	High pressure system design & fabrication, Hypergolic
	propellant handling
Analysis	Cantera (Shock & Detonation Toolbox), ANSYS Fluent
	(Basic Prof.), NUMECA
CAD	SolidWorks, CATIA, Solid Edge
Programming	Matlab, Python (Basic Prof.), C (Basic Prof.)

HONORS AND AWARDS

- Purdue University College of Engineering Nominee, Midwestern Association
 - of Graduate Schools Excellence in Teaching Award, Jan 2019
- Excellence in Teaching Award, Purdue University Graduate School (Nominated), Apr 2018
- 1 of 5 awardees of Magoon Award for Excellence in Teaching, Purdue University, Apr 2019, 2018 & 2015
- Best Presenter Award (of 14 presenters), AAE Research Symposium Series, Purdue University, Apr 2017
- National Science Foundation Travel Grant, US National Combustion Institute Meeting, Apr 2017
- Graduate Teaching Award, Purdue University Center for Instructional Excellence, Apr 2017
- Travel Grant from Purdue Graduate Student Government, Mar 2017

EXPERIENCE

Graduate Research Assistant

Apr 2012 - Dec 2019

School of Aeronautics and Astronautics, Purdue University

- Investigate Deflagration-to-Detonation Transition (DDT) and flame acceleration in Ethylene/Acetylene/Nitrous Oxide and its dependence on initial pressure and ignition energy.
- Evaluate flame acceleration in Acetylene/Nitrous Oxide at different mixture ratios in a 20 ft. open combustion tube.
- Study combustion of a variety of gaseous, liquid and solid fuels with air, by measuring flame speed and pressure to evaluate their tendency to transition to a detonation.
- Study effects of nano-second repetitively pulsed plasma discharges on atmospheric and high-pressure methane/air burners.

Thermal & Fluids Intern for Filtration Research & TechnologyMay2018 - Aug 2018

Cummins Inc., Cookeville, TN

 Development of a method to simulate End-of-Life condition of fuel filters, similar to field returned filters, with respect to Fuel Water Separation (FWS).

- Improve existing End-of-Life conditioning setup.
- Compare FWS performance of new Cummins filter media with that of competitors.

Thermal Engineer for Bipropellant High Energy Stimulation Jan 2013 - Aug 2013

Sandia National Laboratories & EMRTC, NM

- Setup an ethylene-nitrous oxide delivery system for rock formation stimulation using rapid pressurization from detonations.
- Initiation of detonations in formation wellbores based on in-lab detonation experiments conducted at Purdue University.
- Assessment of generated fracture network subsequent to each detonation test based on pressure-time history of wellbore and gas dynamics analysis.

$Undergraduate \ Intern$

Jan 2011 - May 2011

Gas Turbine Research Establishment, Bangalore, India

 Perform CFD analysis of a jet engine intake duct using the commercial CFD software (NUMECA) and compare flow through straight and offset ducts.

Course Projects

School of Aeronautics and Astronautics, Purdue University

- Study the effects of freezing point depression on the density and ignition delay of triethylamine borane with nitric acid (hypergollic green propellants). Aug 2016 Jun 2017
- Design and fabrication of combustor and exhaust management system to test combustion performance of gelled Monomethylhydrazine (MMH) and Red Fuming Nitric Acid (RFNA).
 Jan 2013 - Aug 2013
- Development of fuel estimation, pressure profile and thrust profile codes using ballistic lumped parameter analysis for an LDPE and Hydrogen Peroxide hybrid rocket.
 Jan 2013 - Aug 2013
- Fabrication of Consumable Catalytic Beds (CCBs) which serve as igniters for the LDPE and Hydrogen Peroxide hybrid rocket. Jan 2013 - Aug 2013

JOURNAL PUBLICATIONS

Published/Accepted

- P. Bangalore Venkatesh, J. H. D'Entremont, S. E. Meyer, S. P. M. Bane, M. C. Grubelich, D. King, "Bipropellant High Energy Stimulation for Oil and Gas Applications," *J. Petroleum Science and Engineering, Vol. 180*, June 2019, p. 660-667.
- P. Bangalore Venkatesh, S. E. Meyer, S. P. M. Bane, M. C. Grubelich, "Deflagration-to-Detonation Transition in Nitrous Oxide/Oxygen-Fuel Mixtures for Propulsion," J. Propulsion & Power, DOI: 10.2514/1.B37391, June 2019.

CONFERENCE PROCEEDINGS, PRESENTATIONS & POSTERS

- P. Bangalore Venkatesh, S. E. Meyer, S. P. M. Bane, M. C. Grubelich, "Deflagration-to-Detonation Transition in Pre-mixed Nitrous Oxide - Fuel Mixtures for Propulsion Systems", *1st Amelia Earhart Summit*, Oct 2018, W. Lafavette, IN.
- P. Bangalore Venkatesh, C. Back, A. Liberman, T. Pourpoint, "Freezing Point Depression and its Effects on Density and Ignition Delay of Triethylamine Borane", 53rd AIAA/SAE/ASEE Joint Propulsion Conf., Jul 2017, Atlanta, GA.
- P. Bangalore Venkatesh, T. J. Graziano, S. P. M. Bane, S. E. Meyer, M. C. Grubelich, "Flame Acceleration and DDT in Ethylene/Nitrous Oxide at Elevated Pressures", 10th US National Combustion Meeting, Apr 2017, College Park, MD.
- T. J. Graziano, P. Bangalore Venkatesh, S. P. M. Bane, S. E. Meyer, M. C. Grubelich, "Investigation of Flame Acceleration in Gaseous and Liquid Fuels in the Sandia/Purdue 20 ft. Combustion Tube Facility", 10th US National Combustion Meeting, Apr 2017, College Park, MD.
- P. Bangalore Venkatesh, S. P. M. Bane, "Deflagration-to-Detonation Transition and Flame Acceleration in Nitrous Oxide-Ethylene Mixtures", AAE Research Symposium Series, Mar 2017, W. Lafayette, IN - (Best Presenter Award).

- 4. P. Bangalore Venkatesh, T. J. Graziano, S. P. M. Bane, S. E. Meyer, M. C. Grubelich, "Deflagration-to-Detonation Transition in Nitrous Oxide-Ethylene Mixtures and its Application to Pulsed Propulsion Systems", AIAA SciTech 55th Aerospace Sciences Meeting, Jan 2017, Grapevine, TX.
- M. C. Grubelich, D. King, S. Knudsen, D. Blankenship, S. Bane and P. Bangalore Venkatesh, "An Overview of a High Energy Stimulation Technique for Geothermal Applications", *Proceedings of World Geothermal Congress*, Apr 2015, Melbourne, Australia.
- J. H. D'Entremont, R. Gejji, P. Bangalore Venkatesh, S. P. M. Bane, "Plasma Control of Combustion Instability in a Lean Direct Injection Gas Turbine Combustor", AIAA SciTech 52nd Aerospace Sciences Meeting, Jan 2014, National Harbor, MD.
- P. Bangalore Venkatesh, J. D'Entremont, S. E. Meyer, S. P. M. Bane, M. C. Grubelich, "High-Pressure Combustion and Deflagration-to-Detonation Transition in Ethylene/Nitrous Oxide Mixtures", 8th US National Combustion Meeting, May 2013, Park City, UT.

TEACHING & MENTORING

- Teaching Assistant: Plane Analytic Geometry & Calculus II, Fluid Mechanics Lab, Aerodynamics Labs, Introduction to Fluid Mechanics, Air Breathing Propulsion, Advanced Air Breathing Propulsion, Experimental Aerodynamics, Purdue University.
- Graduate Student Mentor, Purdue Undergraduate Research Experience
 (PURE): Aravinth Chembu, B. Tech. student, IIT Madras, India. May Jul
 2017

PROFESSIONAL ACTIVITIES & SERVICES

School, College, University Service

- Research Group Representative, Zucrow Student Council, Purdue University, Aug 2017 - Present
- Volunteer, Organizing Committee, Inaugural Amelia Earhart Summit, Oct 2018

- Graduate Student Mentor, Aero Assist, Purdue University, 2012 2015
- Judge, Purdue Undergraduate Research Conference Poster Session, Apr 2019 Outreach Activity
 - Scoring Volunteer, MATHCOUNTS nationwide middle school mathematics competition, *Feb 2018 & 2019*

PROFESSIONAL AFFILIATIONS

Aero Assist; Combustion Institute; American Institute of Aeronautics and Astronautics.