Laminar Burning Speeds and Flame Structure Analysis of Gas to Liquid (GTL) Fuel at High Temperatures and Pressures

A Dissertation Presented

By

Mohammed Alswat

To

The Department of Mechanical and Industrial Engineering

In partial fulfillment of the requirement for the degree of

Doctor of Philosophy

In the field of

Mechanical Engineering

Northeastern University
Boston, Massachusetts

April 2017
ACKNOWLEDGEMENTS

First of all, I would like to thank my family for their constant encouragement, continuous emotional support and for their limitless love. To my father who never stopped supporting me in many ways and guided me whenever I needed help. To my mother who never stopped praying for me, supports me and helps me always. To my wife who took a big responsibility of taking care of house, me and my children without complaining and also supporting me all the way.

I am heartily thankful to Professor Hameed Metghalchi for first accepting me in his team, introduced me to his research, guided me through this experimental investigation and answering all my questions. He was like a father to me and always reminded me that health comes first, then family and last is work. I will never forget his support when I had some health issues which was the toughest time in my life. Thank you for your guidance, patience, encouragement and continuous moral support during the course of this work. I feel honored and blessed at the same time to have the opportunity to work with you.

I would like to thank my dissertation committee members: Professor Reza Sheikhi and Professor Mehdi Abedi for their time, interest and feedbacks. I would like to express my sincere gratitude to all my teachers at Northeastern University: Professor Mohammad Taslim, Professor Behrooz Satvat, Professor Uichiro Narusawa, the late Professor Yaman Yener, and Professor John Cipolla, thank you all.

My thanks to Northeastern University, specifically the Mechanical and Industrial Engineering Department for the educational opportunities provided by the faculty and staff through my years of study. Finally, I would like to thank my team who helped me a lot in the laboratory.
My thanks to Dr. Omid Askari, Kevin Vien, Ziyu Wang, Moaz Allehaibi and Guangying Yu.
Especial thanks to my two best friends in Boston Emad Rokni and Abdulsami Aldahlawi for their support and help.
List of Figures

Figure 1: Cylindrical combustion vessel ................................................................. 12
Figure 2: Cylindrical combustion vessel side view .................................................. 13
Figure 3: Exploded view of cylindrical vessel ....................................................... 13
Figure 4: Spherical combustion vessel ................................................................. 14
Figure 5: Exploded view of spherical vessel ......................................................... 15
Figure 6: The gas manifold ................................................................................... 16
Figure 7: Liquid fuel injection system ..................................................................... 17
Figure 8: Spark plug electrode image ..................................................................... 20
Figure 9: Shadowgraph system layout ................................................................. 22
Figure 10: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 0.5$ atm ................................................................. 27
Figure 11: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 1.0$ atm ................................................................. 28
Figure 12: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 2.0$ atm ................................................................. 29
Figure 13: Snapshots of GTL/air flames at five different equivalence ratios and three different initial pressures, $T_i = 490$ K ................................................................. 30
Figure 14: Typical pressure output file from experimental run, $T_i = 490$ K, $P_i = 2.0$ atm, $\varphi=1.0$. .................................................................................................................. 32
Figure 15: Schematic of different zones and their corresponding temperatures in the thermodynamics model ................................................................. 33
Figure 16: Unburned gas conditions along an isentrop for $\varphi=1$ ........................... 40
Figure 17: Unburned gas initial conditions along an isentrop for $\varphi=1$ ................................. 40

Figure 18: Laminar burning speed versus stretch rate for GTL/air mixture ......................... 41

Figure 19: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\varphi = 0.7$ ........................................................................................................................................ 43

Figure 20: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\varphi = 0.85$ ........................................................................................................................................ 44

Figure 21: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\varphi = 1.0$ ........................................................................................................................................ 44

Figure 22: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\varphi = 1.12$ ........................................................................................................................................ 45

Figure 23: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\varphi = 1.2$ ........................................................................................................................................ 45

Figure 24: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i = 490$ K, $P_i = 0.5$ atm ................................................................................................. 46

Figure 25: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i = 490$ K, $P_i = 1.0$ atm ................................................................................................. 46

Figure 26: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i = 490$ K, $P_i = 2.0$ atm ................................................................................................. 47

Figure 27: Laminar burning speeds of GTL-air flames for different pressures, equivalence ratios and $T_i = 490$ K ........................................................................................................ 47

Figure 28: Comparison of measured laminar burning speeds of GTL-air with other reported values at $T=490$ K and $P=1$ atm as a function of fuel/air equivalence ratios .......... 48

Figure 29: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, $T = 490$ K and $P = 1.0$ atm ................................. 49
Figure 30: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, $T = 490$ $K$ and $P = 0.5$ $atm$ .............................................. 49

Figure 31: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, $T = 490$ $K$ and $P = 2.0$ $atm$ ............................................. 50
List of Tables

Table 1: Specification properties of GTL S-8 fuel......................................................... 4

Table 2: Laminar burning speeds of common fuels at room temperature T= 300 K, 1
atmospheric pressure, and stoichiometric ................................................................. 9

Table 3: Fitted parameters for GTL burning speeds correlation....................................... 42
Abstract

Laminar burning speed and flame structure of gas-to-liquid (GTL) fuel has been experimentally measured and analyzed using cylindrical vessel. Since GTL is a mixture of many hydrocarbons, all of the experiments have been done at high temperatures when most constituents have been evaporated. A novel liquid injection system with heating elements have been used to evaporate the liquid fuel before entering to the combustion vessel. Shadowgraph system and a high speed camera that can take up to 40,000 frame per second pictures are set up with the cylindrical vessel to capture the optical recordings of the combustion event. This allows us to observe the flame structure and to investigate the onset of instability.

Laminar burning speeds of mixture of GTL/air have been measured in the cylindrical vessel. The dynamic combustion pressure measured in the cylindrical vessel is the input for the burning model to calculate burning speed. The thermodynamic model used to calculate the burning speed from the pressure rise includes the radiation losses from burned gas to the wall of the vessel, temperature gradient in preheat zone, energy loss to electrodes and convective energy loss to the wall. NASA polynomial coefficients has been used in the model to calculate the unburned gas properties while STANJAN code was used for the burned gas properties calculation.

Burning speed of GTL/air mixture have been measured for initial temperature of 490 K and a wide range of pressures and equivalence ratios. Power low correlation for burning speed of GTL/air mixture has been developed that is valid in the range of \(0.7 < \varphi < 1.2\), \(490 K < T < 620 K\), \(0.5 atm < P < 4.3 atm\). Based on the burning speed results, it was noted that the laminar burning speed is proportional directly to temperature and inversely to pressure.
Table of Contents

ACKNOWLEDGEMENTS ........................................................................................................... i
List of Figures .......................................................................................................................... iii
List of Tables ............................................................................................................................ vi
Abstract .................................................................................................................................. vii

1. Introduction .......................................................................................................................... 1
  1.1. Background .................................................................................................................... 1
  1.2. Literature review ........................................................................................................... 5
  1.3. Determination of the Laminar Burning Speed .............................................................. 6
      1.3.1. Computational Method ..................................................................................... 6
      1.3.2. Experimental Method ..................................................................................... 7
  1.4. Statement of the Problem ............................................................................................ 9

2. Experimental Facility and Methods ................................................................................... 11
  2.1 Cylindrical Vessel .......................................................................................................... 11
  2.2 Spherical Vessel ............................................................................................................ 13
  2.3 Gas Manifold ................................................................................................................ 15
  2.4 Liquid Fuel Injection Systems ....................................................................................... 16
  2.5 Heating Systems ........................................................................................................... 18
  2.6 Ignition System ............................................................................................................ 18
      2.6.1 Ignition Power Box ............................................................................................ 19
      2.6.2 Transformer Circuit ............................................................................................ 19
      2.6.3 Spark Plug Electrodes ....................................................................................... 20
  2.7 Ionization Probes ........................................................................................................... 21
  2.8 Shadowgraph Setup ...................................................................................................... 21
  2.9 Data Acquisition System ............................................................................................... 22
  2.11 Experimental Procedure ............................................................................................. 23

3. Flame Structure and Thermodynamic Model .................................................................. 25
  3.1. Flame Structure and instability ................................................................................... 25
  3.2. Thermodynamic Model ............................................................................................... 31
      3.2.1. Assumptions ..................................................................................................... 32
      3.2.1. Burned Gas Mass Fraction and Temperature ................................................... 33
      3.2.2. Burning Speed ................................................................................................. 36

4. Results ................................................................................................................................. 38
  4.1. Stretch Effects .............................................................................................................. 38
4.2. Laminar Burning Speeds Results ................................................................................. 41
4.3. Comparison .................................................................................................................. 48
5. Summary, Conclusions and Recommendations ............................................................ 51
6. References ....................................................................................................................... 53
Appendix A: Laminar burning speed code .............................................................. Error! Bookmark not defined.
1. Introduction

1.1. Background

Laminar burning speed is defined as the speed at which a planar, one-dimensional, adiabatic flame travels relative to the unburned gas mixture. Laminar burning speed of homogenous fuel, oxidizer, diluent gas mixtures are considered the most essential factors for developing and testing out chemical kinetic models of hydrocarbon oxidation. Laminar burning speed also has been used extensively in direct practical applications in the fields of engines, burners, explosions and chemical processors. In practice, the laminar burning speed is an essential physicochemical property of premixed ignitable gases, and a function of pressure, temperature, fuel/air equivalence ratio and diluents compositions. The laminar burning speed directly determines the rate of energy released during the burning of combustible gas mixtures. Besides, it is a primary parameter in common models of turbulent combustion as well as wall quenching [1-3].

In the validation of numerical codes or assessment of combustion theories, it is important to have measurements for the laminar burning speed. The accuracy is even more important when the assessment involves heavy hydrocarbon fuels normally used for internal combustion engines. Other primary uses of the laminar burning speed include the prediction of the burning rates of fuel and the calibration or validation of chemical reaction mechanisms. In Keck’s [1] model for turbulent flame propagation and pollution formation in internal ignition engines, he used the laminar burning speed. In a different turbulent combustion model, Karpov et al [4] opted for the laminar combustion speed as the sole input parameter for the study. When calculating the performance of internal combustion engines or gas turbines, it is
important to know the laminar combustion properties of liquid fuels burning at higher temperatures. In order for scientists to predict how engines operate and perform, there is need for additional parameters such as wall quench layer thickness, minimum ignition energy, and laminar burning speed as the frame of reference. Wall quench layer thickness is described as the boundaries existing near physical geometry that have gas properties that do not support burning and is related to temperature and energy transfer. The minimum ignition energy refers to the least quantity of energy input needed to support combustion which is related to the laminar burning speed. Another significant application of the laminar burning speed data involves lowering combustion emissions and improving efficiency of vehicle engines and gas turbines. In particular, measuring the laminar burning speed at high pressure and temperatures conditions is critical when one seeks to analyze and predict the performance of power plants or internal combustion engines. In the modern world, new fuels are entering the marketplace yet people know little about them. Accordingly, it is challenging and time consuming to find the chemical reaction mechanisms for these fuels. Fortunately, the availability of the laminar burning speed is helpful and necessary to validate and calibrate the mechanisms. Lastly, it is not as easy to measure the laminar burning speed for liquid fuels as it is for gaseous fuels. The process of vaporizing the liquid fuel and mixing it in the right proportions with an oxidizer often involves a host of challenges.

Due to supply security and environmental impact, finding an alternative to oil-based transportation fuel is very important now than ever. Synthetic Paraffinic Kerosene (SPK) fuels is an alternative fuel obtained from coal, biomass and natural gas. Since using SPK as an alternative fuel does not require a modification to exciting fuel injection/combustor system, it was gained a lot of interest especially for aviation transportation. The SPK fuels are a composition of normal-alkanes, iso-alkanes and cyclic-alkanes which is produced using Fisher-
Tropsch (F-T) process. Among SPK fuels, gas-to-liquid (GTL) fuel is having the most interest from aviation because of it is cleaner combustion characteristics due to the near absence of sulfur [5].

The Air Force Research Laboratory (AFRL) has provided Northeastern laboratory with the GTL fuel and its detailed composition, S-8 [6]. The surrogates of GTL that used in this study are a blend of 32% of iso-octane, 25% n-decane and 43% n-dodecane. This surrogate mixture has an empirical formula of $C_{10.22}H_{22.44}$, H/C ratio of 2.196 and a molar mass of 145.37 g/mol.

The initial mixture composition for GTL/air mixture is defined as:

$$\varphi (0.32C_8H_{18} + 0.25C_{10}H_{22} + 0.43C_{12}H_{26}) + 15.83(O_2 + 3.76N_2) \ldots \ldots \ldots (1.1)$$
<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial boiling point (K)</td>
<td>426</td>
</tr>
<tr>
<td>10% recovered (K)</td>
<td>444</td>
</tr>
<tr>
<td>20% recovered (K)</td>
<td>453</td>
</tr>
<tr>
<td>50% recovered (K)</td>
<td>481</td>
</tr>
<tr>
<td>90% recovered (K)</td>
<td>520</td>
</tr>
<tr>
<td>Final boiling point (K)</td>
<td>533</td>
</tr>
<tr>
<td>Flash point (K)</td>
<td>321</td>
</tr>
<tr>
<td>Freezing Point (K)</td>
<td>222</td>
</tr>
<tr>
<td>Density @ 15°C (kg/L)</td>
<td>0.75</td>
</tr>
<tr>
<td>Viscosity @ -20°C (mm²/s)</td>
<td>4.3</td>
</tr>
<tr>
<td>Net heat of combustion (MJ/kg)</td>
<td>44.1</td>
</tr>
<tr>
<td>Conductivity (pS/m)</td>
<td>128</td>
</tr>
<tr>
<td>Lubricity test (BOCLE) wear scar (mm)</td>
<td>0.59</td>
</tr>
<tr>
<td>Aromatics (% vol)</td>
<td>0.0</td>
</tr>
<tr>
<td>Total sulfur (% mass)</td>
<td>&lt; 0.0003</td>
</tr>
<tr>
<td>Hydrogen content (% mass)</td>
<td>15.4</td>
</tr>
</tbody>
</table>

**Table 1: Specification properties of GTL S-8 fuel**

As mentioned earlier, Fischer-Tropsch (F-T) fuels are of increased interest as alternative jet fuels. However, combustion and emission characteristics of different F-T fuels are not yet studied in sufficient details [7]. It is very important to understand these characteristics in order to consider them as a potential replacement of conventional jet fuel such as Jet-A.
1.2. Literature review

Kick, et.al. [8] measured the laminar burning speed of GTL and GTL+20% hexanol fuel at atmospheric pressure and different preheat temperatures by using the cone angle method.

Ji, et.al. [9] determined laminar burning speeds and extinction strain rates of premixed S-8/air, Shell-GTL/air, R-8/air, JP-7/air, and JP-8/air flames at atmospheric pressure for $0.7 \leq \phi \leq 1.5, T_u = 403K$. They also determined extinction strain rates of nonpremixed flames of S-8, Shell-GTL, R-8, JP-7, JP-8, n-decane, and n-dodecane/air.

Kick, et.al. [10] measured the laminar burning speeds of three GTL-air synthetic fuel-air mixtures and a coal to liquid (CTL) fuel at ambient pressure and at a preheat temperature of 473K, for $1.0 \leq \phi \leq 1.4$. It also compared with Jet A-1 which measured earlier by Eberius [11] in a similar burner test rig for $1.1 \leq \phi \leq 1.4$.

Wang, et.al. [12] measured ignition delay time for Jet A, Jet A+JP-8, S-8, Shell GTL, Sasol IPK fuel/air mixtures at equivalence ratios from 0.25 to 1.5 for 651-1381 K and 8-39 atm.

Vukadinovic, et.al. [13] measured the laminar burning speeds of kerosene Jet A-1, GTL, and GTL+ aromatics at three different initial temperatures, 100 °C, 150 °C, and 200 °C and three different initial pressures 1, 2, and 4 bar for a wide range of equivalence ratios between 0.66 and 1.66 by using a two-dimensional Mie-scattering laser light method.

The experiments by Eigenbrod, et.al. [14] have been carried out in a hot blow-down wind-tunnel to investigate the ignition behavior (e.g. auto ignition) of a GTL kerosene by Shell at the pressure range between 4.5 and 6 bar and at temperatures ranging from 740 to 840 K.

Dagaut, et.al. [15] investigated oxidation kinetics by using a JSR (at p=10 bar and a constant mean residence time of 1 s, $770k < T < 1070k$, and for variable equivalence ratios $0.5 < \phi < 2.0$), ignition delay time by using a shock tube (at p around 16 bar, $650k < T < 1400k$,
φ = 0.5 and φ = 1.0), laminar burning speed by a conical flame burner (at p= 1 bar and a preheat temperature of 473 K, φ = 1.0-1.5) with the diluent of Nitrogen.

Dagaut, et.al. [16] studied the oxidation kinetics of a GTL jet fuel blended with hexanol in JSR (at p=10 bar, a constant mean residence time of 1 s, 550K < T < 1150K, 0.5 < φ < 2.0).

Mzé-Ahmed, et.al. [17] studied the oxidation kinetics of a GTL synthetic jet fuel and a GTL/1-hexanol blend synthetic jet fuel in JSR (at 10 bar, a constant mean residence time of 1 s, between 550 and 1150 K, and over a range of equivalence ratios (0.5–2.0). The conditions are same as before except for a diluent of Nitrogen.

In these studies, the lowest operating temperature for calculating laminar burning speed was 373K and the highest was at 473K. since those experiments were below 50% evaporation rate as listed in table 1, in this study the initial temprature of the mixture were increased.

1.3. Determination of the Laminar Burning Speed

Numerical simulations and experimental methods are the two main methods of determination of laminar burning speed.

1.3.1. Computational Method

Numerical simulations of laminar flames involve carrying out in-depth consideration of chemical kinetics, thermo-chemical property, as well as the exact and simplified transport formulations to be used with solution of governing differential equations [18-19]. Originally, shooting techniques were the earliest attempts to solve premixed flame problems with realistic chemical kinetics [20-21]. Unfortunately, the complex nature of kinetics made those techniques unusable. The GAMM workshop, by Peters and Warnatz [22] as well as Kendal and Kelly [23], summarizes the majority of early work done on premixed flame modeling. The summary
introduces the idea of solving steady state problems through finite-difference boundary-value-problem methods.

1.3.2. Experimental Method

Different experimental methods have been used to determine the laminar burning speed. Researchers such as Linnett [24], Andrews et al [25], and Rallis et al [26] prepared excellent reviews of previous measurements for laminar burning speeds. There are two primary methods for measuring the burning speeds. The first method involves stationary flames such as the Bunsen burner and nozzle burner flames. The second method involves propagating flames of freely spherical flames and propagating flames via flame tubes. In the current investigation, the researcher uses the freely/outwardly expanding spherical premixed flame configuration for measurements. The first category includes both diffusion and premixed flames. Examples of diffusion flames include burning candles, wood, or coal. Examples of premixed flames include the flame of the Bunsen burner.

Some researcher used the burner method to obtain laminar burning speed [27-30]. In these studies, researchers used the burner methods because they involve inexpensive, versatile, but superficially easy to use apparatus. Unfortunately, the majority of results obtained through these methods are doubtful [26]. The main disadvantage of the burner methods include lack of uniformity of the burning speed over the flame surface, that is, the flame tip and burner rim due to energy transfer to the rim. In addition, another disadvantage involves difficulty in establishing the relevant unburned gas temperature profile through any section of flame. In practice, constant pressure experiments based on flat flame burners are always limited to a narrow range of temperatures. In most cases, they are useful to obtain data at the atmospheric pressure.
Propagating flames method are either constant volume [31-43] or constant pressure [44-63] techniques. In the constant pressure method by Law and coworkers [31, 34-35, 40], they used a cylindrical double-vessel. In this apparatus, the inner vessel wall is characterized by a few rows of holes which are covered using a sleeve mechanism. When the pressure in the inner vessel increases, the sleeve is displaced and part of the gas escapes to the outer vessel via the holes, and, therefore, ensuring that constant pressure is maintained within the inner vessel.

Also, Bradley and coworkers [39, 41, 43] utilized a larger spherical vessel which had optical access. However, they limited their calculations to the start point of the combustion since the increase in pressure is negligible. Based on the size of the vessel, they can get sufficient data point for analysis. The major shortcoming associated with constant pressure experiments is that they provide data for only a single condition for each experiment. Besides, these experiments will need substantial corrections for stretch effect since flame radii are small.

Unlike the constant pressure methods, the constant volume approach will cover a broad range of temperatures and pressures [45, 54]. In addition, the propagating flame will provide a range of data on an isentrope in a solo experimental run. Moreover, the constant volume method is easy to build the experimental facilities and to conduct the experiment. Many studies [45, 48-54] utilized the spherical combustion chamber approach to determine the laminar burning speed for a wide range of fuels, diluent concentrations, temperature, and pressures. Lastly, the following is a table outlining the laminar burning speeds of common fuels used at room temperature T=300 K, 1 Atmospheric pressure, and equivalence ratio of 1 [41].
1.4. Statement of the Problem

Even though numerous studies have been done on burning speed measurements of premixed fuels at room temperature and atmospheric pressure little focus is often paid to the same measurements at higher temperatures and pressures. Besides, as newer fuels and hydrocarbon blends continue to penetrate the marketplace, there is greater need to determine the fundamental properties of these fuels especially the burning speed. Numerical calculations involving commercial codes such as Sandia PREMIX codes and CANTERA are useful in calculating the burning speed. However, the codes depend on models for chemical kinetics that are absent for heavy hydrocarbons. Due to lack of complete chemical kinetics and transport properties, the numerical calculation result in inaccurate predictions of the burning speed. As mentioned previously, it is important to validate and calibrate chemical reaction models using experimental data. In the subsequent chapters, the author discusses theoretical model to

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Laminar Burning Speed (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane (CH₄)</td>
<td>36</td>
</tr>
<tr>
<td>Acetylene (C₂H₂)</td>
<td>136</td>
</tr>
<tr>
<td>Ethylene (C₂H₄)</td>
<td>67</td>
</tr>
<tr>
<td>Ethane (C₂H₆)</td>
<td>43</td>
</tr>
<tr>
<td>Propane (C₃H₈)</td>
<td>44</td>
</tr>
<tr>
<td>Hydrogen (H₂)</td>
<td>210</td>
</tr>
</tbody>
</table>

Table 2: laminar burning speeds of common fuels at room temperature, 1 Atmospheric pressure, and equivalence ratio of 1
determine burning speed from pressure rise due to combustion of fuel/air mixture in a constant volume vessel.

Recently, the development of viable alternative aviation fuels has attracted much interest, for many reasons, with reduction of greenhouse gas (GHG) emission and ensuring security of supply at affordable price among them. GTL fuel is clean when it is compared to crude oil. It contains almost none of the impurities (nitrogen and sulfur). Currently there is not many data on the laminar burning speed of GTL in literature especially at high temperatures and pressures.

In this research laminar burning speed of GTL/air mixture supplied from Air Force Laboratory, known as S-8, is measured for temperature range of $490 \,{\text{K}} < T < 620\,{\text{K}}$, pressures ranges of $0.5\,\text{atm} < P < 4.3\,\text{atm}$ and equivalence ratio $0.7 < \varphi < 1.2$. Chapter 2, 3 and 4 describes Experimental Facility and Methods, Flame Structure and Thermodynamic Model and the Results.
2. Experimental Facility and Methods

A full description of the experimental apparatus used in the study is presented in this chapter. The majority of the apparatus were designed and constructed in the laboratory. These apparatus include combustion chambers, gas manifold, ignition system, and liquid injection lines and heaters.

2.1 Cylindrical Vessel

The cylindrical vessel can be seen in Figures 1 - 3. It is made from 316 SS and has a diameter of 13.5 centimeters and height of 13 centimeters. The cylindrical vessel has Pyrex windows of 3.5 centimeters thickness at each end. The ends are sealed to the chamber using O-rings. These windows enable the vessel to function up to a maximum pressure of 50 atmospheres. Thicker windows can be insulated in order to increase the maximum allowable pressure. The main function of the windows is to ensure a clear line of sight via the vessel so as to accommodate a Shadowgraph setup that allows for real-time observation and recording of the combustion event. The chamber is fitted with ports for spark electrodes and port for filling and evacuating the chamber. The cylindrical vessel also has fittings of similar spark plugs with extended electrodes to enable center point ignition. It also has thermocouples for measuring the internal temperature of the chamber and the walls of the vessel. The cylindrical vessel is fitted with band heaters to facilitate heating of the vessel to 500K—this is the limit of the elastomer O-rings.
Figure 1: Cylindrical combustion vessel

Figure 2: Cylindrical combustion vessel side view
The spherical vessel shown in Figures 4 and 5, was made from two hemispheres bolted together to create a perfect sphere having a diameter measuring 15.24 centimeters. The material used in making the hemisphere is the 4140 steel of thickness 2.54 centimeters. This enables the hemispheres to sustain internal pressures of up to 425 atmospheres if they are bolted together using the 8 bolt locations. The spherical vessel has access ports comparable to those of the cylindrical vessel. A tube measuring 6mm at the bottom of the vessel is used in filling and evacuating the vessel. Also, the vessel has fittings of two extended spark plug electrodes. These electrodes offer a center point ignition source for the chamber. The Kistler 603B1 piezoelectric pressure transducer fitted in one of the chamber ports as well as a Kistler 5010B charge amplifier are utilized to record the dynamic pressure vs. time records used for determining the
burning speed. In addition, the chamber is fitted using two thermocouples that are used to measure the internal temperature and temperature of the outer wall. At the flush, three ionization probes are mounted to measure the arrival time of the flame at the wall and check the spherical symmetry and buoyant rise. The whole vessel is in a large oven that can elevate the vessel’s temperature to ~700 K. however, it is important noting that the O-rings that seal the two hemispheres have temperature limit of 500K.

Figure 4: Spherical combustion vessel
2.3 Gas Manifold

The gas manifold can be seen in Figure 6. It is an auxiliary system for attaching to the spherical and cylindrical vessels. The purpose of the gas manifold is to distribute the gaseous fuels, diluents, and oxidants to the systems and at the precise pressures. Also, the gas manifold creates a common path to the vacuum pump. The three gauges provide measurement for the pressure of the constituent being metered to a specific vessel. One of the pressure gauges is a thermocouple type gauge designed to measure very low pressures aimed at verifying near perfect vacuum. A second gauge is a piezoelectric pressure transducer designed to measure a maximum of 15 psia. Finally, the last gauge is a piezoelectric transducer that measures up to 250 psia. Both the manifold and the system are connected to a vacuum pump capable of achieving 1 micron of vacuum when functioning properly. The right gauges are used successively as the partial filling pressure increases until one attains the right filling pressure.
2.4 Liquid Fuel Injection Systems

Each of the combustion vessels are fitted with identical liquid fuel injection systems. A diagram of the injection system is in figure 7. In the system, the liquid fuel injection system is located close to the main valve of combustion vessel so that it can minimize the volume piping between the fuel source and the vessel. An injection system is made of a fuel reservoir, fuel inlet valve, safety check valve, piezoelectric transducer, and an arrangement of valves. The safety check valve serves the function of protecting the transducer while the arrangement of valves serve the purpose of isolating the injection system and the bomb from the gas manifold piping and the piping resistive heaters that are embedded to the metallic hemisphere surrounding the piping.
The entire injection system piping is heated at least 490 K for the purposes of maintaining the fuel in a vaporized state as it moves through the vessel. During this time, a Kulite temperature controller is used to monitor the temperature along the line. Also, the fuel reservoir of the injection system is full of appropriate fuel whose temperature is equivalent to the room temperature.

The fuel valve and remaining components of the system are treated to reasonable temperature increase and left under very low vacuum. With fuel at 1 atmosphere relative to a very hot piping system, the fuel valve is open for fuel to be drawn into the system and is flash boiled to enable the whole fuel vaporizes. The vaporized fuel moves in the vessel as the temperature is monitored using a pressure transducer attached to the line. After obtaining the correct pressure, the vessel valve remains closed, the filling line vacuum pumped, and the vessel is now ready for the addition of oxidizers through the manifold piping system. Using this
method to fill the vessel with liquid fuel vapor is accurate and efficient compared to previous methods [47].

2.5 Heating Systems

Both the cylindrical and spherical vessels have heat capacities of up to ~500 K to allow the experiment to be carried out at high temperatures. In the cylindrical vessel, the temperature is achieved using a cylindrical oven having a diameter of 55 centimeters and height of 65 centimeters. The oven completely encapsulates vessel; its heat source include two 5kW resistive heaters encased on the ceramic walls of the oven. Two 1.5 kW band heaters also heat the cylindrical vessel. The two band heaters are bolted on the flanges of the vessel. The exposed areas of the cylindrical vessel are insulated properly to facilitate even distribution of heat/temperature on the walls of the vessel. Each of the injection systems fitted to the vessel have 1.1 kW heaters to heat the piping from the fuel reservoir to the vessel. The heating at these points is to ensure that the fuel remains in a vaporized state.

2.6 Ignition System

The ignition system must be redesigned so that it can deliver consistent quantity of energy to the combustible mixture in a repeatable manner. Its design also includes five unique settings to enable the users deliver from ~ 52mJ of energy to ~ 420mJ of energy. This energy helps in activating the reaction. The ignition system is made up of a new power output box, automotive transformer circuit, and extended automotive spark plugs. DC pulse is delivered to the transformer circuit by the ignition power box. Once delivered, the DC pulse generates a high voltage potential across the spark plug gap. This high voltage breaks down to a certain
voltage to produce a spark needed to initiate combustion. The following subsections provide in-depth information on the subcomponents of the ignition system.

2.6.1 Ignition Power Box

The diagram of the ignition power box is in figure 9. An isolated AC source from an isolation transformer powers the ignition power box. In this case, isolation is very important to prevent stray voltages from finding access to any sensitive equipment being used in the laboratory. The ignition power box then converts the AC power into DC power which is divided into five settings from 20 volts to 120 volts by the simple voltage divider available in figure 9. After selecting the appropriate voltage, a capacitor of 100μF is given a charge of the same voltage to make the system ready to fire. A trigger signal is sent from the data acquisition system through an optical isolator and closes the triac that connects the negative terminal of the capacitor to the output ground. Once the triac is closed, the charged capacitor is coupled to the output of the power box before the DC pulse is released to the transformer circuit.

2.6.2 Transformer Circuit

The transformer circuit accepts the DC pulse originating from the power box. Thereafter, a simple mutual inductance process enables it in a ratio of 1:100. Accordingly, the transformer will produce approximately 3000V which is sent to the electrodes of the selected vessel to generate a spark.
2.6.3 Spark Plug Electrodes

The spark plug electrodes comprise two automotive type spark plugs. These automotive spark plugs have their ground prongs filed off as shown in figure 8. The central electrode is extended by welding a 0.4 mm diameter stainless steel wire to the electrode so that it can reach the center of the vessel. Once produced, both electrodes are installed and set at 0.76mm apart. In experiments, the small diameter electrodes are effective and can minimize heat transfer from the combustion event to the electrode material. An analysis on the heat loss to the electrodes is in the subsequent chapters.

Figure 8: Spark plug electrode image
2.7 Ionization Probes

Ionization probes refer to devices that are used in pin pointing the arrival of the flame front to the vessel wall. Ionization probes function on the simple basis that when gases ionize, they become good conductors of electricity. In this case, the probes take advantage of the ionized gases in the flame front to detect the arrival of the flame. Ionization probes are made of a bolt threaded onto the vessel that has an electrically insulated pin in the core of the bolt. The end of the pin is in proximate distance to the bolt material which is flush to the vessel inner wall when installed. When the ionized gases in the flame pass through the space between the ground and pin, current flows through the circuit and produces signal which is then relayed to the data acquisition system.

2.8 Shadowgraph Setup

This system is set up with the cylindrical vessel to capture the optical recordings of the combustion event. As shown in figure 9, the Z-type shadowgraph/schlieren set [63] has 5 components. The light source is a 10-Watt Halogen lamp having a condensing lens and small pinhole measuring 0.3mm in diameter. It provides a sharp and intense illumination in the entire system. The pinpoint source of light is captured by a spherical mirror with one-eighth wavelength of surface accuracy 152.4cm away that reflects the parallel light rays in a 15.24cm circular beam travelling via the combustion bomb to the spherical mirror in the opposite side. As soon as the circular pattern falls on the second mirror, it is again focused onto a pinpoint that is 152.4cm away onto a CCD camera of high speed (1108-0014, Redlake Inc.) and capture rate of approximately 40,000 frames each second. The research can vary and optimize the camera’s capture rate and shutter speed on the basis of burning speed of the mixture as well as brightness of the flame. The image received by the camera with shadowgraph system in place
is highly sensitive to density variation, and, therefore, can allow us to study the changes in density of the mixture when the combustion is taking place. The detailed analysis of the optics expanding spherical flames and other pictures of flames are presented in the next sections.

Figure 9: Shadowgraph system layout

2.9 Data Acquisition System

This system serves the purpose of recording the pressure-time data and signals generated from ionization probes. In addition, it initiates the combustion event. In order to calculate the correct partial pressures needed to fill the vessels with the correct portions of fuel and oxidizers, one uses the excel sheet code in which the fuel, oxidizer, and diluents are balanced chemically; the partial pressures can be calculated through mole fractions for each species in the balanced equation. The vessel devices are the piezoelectric pressure transducer, two thermocouples, and three ionization probes. The Kistler amplifier amplifies the signal
originating from the pressure transducer. It converts it from the 4-20mA signal into a 10mV/psia signal which is then transmitted to the analogue to digital conversion box.

Knowing the concentrations of different species in the blended fuels is very important during the experiment. In this case, using the Varian Gas Chromatograph with the Varian Hydrogen Generator is recommended. The two tools are incorporated in the laboratory for the purposes of determining the concentration of gaseous and liquid species such as carbon monoxide, carbon dioxide, alkanes, alkenes, alkynes, and oxides of nitrogen in the products or complex liquid fuels such as GTL. Based on analysis with the Gas Chromatograph on fuel blends such as GTL, it is clear that the composition of the fuels will vary from one manufacturer to another. Accordingly, it is important to consider these different when analyzing the data from the experiment.

2.11 Experimental Procedure

The test procedure commences by evacuating the vessel and gas handling system through the use of the vacuum pump. Thereafter, fuel vapor is filled into the chamber to the desired pressure and sealed from the gas manifold using the chamber shut-off valve. Once this is done, the feeding line is evacuated to eliminate excess fuel molecules out of the line. Lastly, the oxidizer and other diluents are added to the mixture. This is done based on the desired pressure and in order of the respective partial pressures. The vessel as well as the fuel tank should be at the same temperature when being filled. Once the chamber is full with the appropriate mixture, it is important to wait for several minutes to allow the system become quiescent before the ignition. This step is important to prevent any potential turbulence inside the vessel.
There are two thermocouples on the liquid line. These thermocouples are important to ensure that the temperature level at the filling line does not fall below the condensation temperature for vaporized liquid fuels. Similarly, it is essential to monitor the partial pressure of fuel throughout the filling process. These considerations are critical because any slight condensation of vaporized fuel will cause a drop in the pressure values as read on the pressure gauges. Alert on the gauges will demonstrate that gasification has failed to a certain degree.

Again, the excel sheet code is used in calculating the partial pressures of fuel, oxidizers, and diluents. It also helps in calculating mole fractions of components in the mixture through chemical balancing of the corresponding reactions. To achieve a reliable statistical sample, it is advisable to make at least three runs for each initial condition. Following the statistical analysis of the data, three runs are adequate for one to achieve a 95% confidence level [64].

The measurements for burning speed were restricted to flames that had a diameter of at least 3.8 cm and in which the flame stretch effects are negligible. In such conditions, the pressure is approximately 5-10% greater than the initial value, and, therefore, the pressure method is useful in calculating burning speed. The wrinkles and instabilities of the flame can be detected using motion pictures captured in the cylindrical chamber.
3. Flame Structure and Thermodynamic Model

Flame structure and the thermodynamic model that used to calculate laminar burning speed from measured combustion process is described in this chapter. The model has been adapted in relation to earlier works [47, 55], and includes few corrections.

3.1. Flame Structure and instability

Flame structure and instability study for GTL/air flame is described in this section. Instability of the flame, in this study means when the flame transits from smooth to cellular. This transition of the flame can be studied and inspected from the pictures that are taken using high speed camera that used to capture the flame propagation. The instability can be categorized into two significant category, thermos-diffusive and hydrodynamic instabilities in terms of effective Lewis number and flame thickness [66].

Lewis number (Le=α/D) determines the thermo-diffusive instability. The flame front should be stable unless if the thermal diffusively \( \alpha_{th} \) of the mixture is sufficiently less than the mass diffusivity \( D_m \) of the reactant [70].

The gas expansion which results from the energy released by chemical reaction is the cause of the hydrodynamic instability. This energy released from the chemical reaction induces a flow that tends to make any flame perturbation further away from the original shape. The thermal expansion ratio \( \sigma \) which directly affect the growth rate of the hydrodynamic disturbance is defined as the ratio of the unburned density (\( \rho_u \)) to the burned density (\( \rho_b \)) of the mixture [71]. This ratio is about 7 and increases small perturbation of flame front makes it cellular and unstable.
Burning speed measurements have been done only for smooth flames. Therefore, it was not necessary to include data from cellular flames into calculations. Flame structures of all conditions have been studied and the critical conditions at which cell formations occurred were identified by using optics. Figures 10-12 show the snapshots of GTL/air flames for three different initial pressures at five equivalence ratios and initial temperature of 490 K. Figure 13 shows the snapshots of GTL/air flame when it hits the wall for three different initial pressures at five equivalence ratios and initial temperature of 490 K. As it can be seen in the figures as flame radii and pressure increase the tendency of flame cellularity increases.

As shown in Figure 10, it was noted that when the initial pressure is $P_i = 0.5 \text{ atm}$, the flame is smooth for both lean and rich mixtures. While for $P_i = 1.0 \text{ atm}$ as shown in Figure 11, the flame is smooth when the mixture is lean and partially smooth for stoichiometric and rich mixtures. As the pressure increase to $P_i = 2 \text{ atm}$, Figure 12, the flame is completely smooth for $\phi = 0.7$, partially smooth for $\phi = 0.85$ and $\phi = 1$ and completely cellular for rich mixtures.
Figure 10: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 0.5$ atm
Figure 11: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 1.0$ atm
Figure 12: Snapshots of GTL/air flames at five different equivalence ratios, $T_i = 490$ K, $P_i = 2.0$ atm
Figure 13: Snapshots of GTL/air flames at five different equivalence ratios and three different initial pressures, $T_i = 490$ K
3.2. Thermodynamic Model

The thermodynamic model utilized in calculating the burning speed from the pressure rise is related to the one originally developed by Metghalchi and coworkers [47, 55]. Figure 14 shows an example of the pressure vs time during a combustion process. The pressure signal shows that the flame hits the wall at about 0.025 sec. Flame is in contact with the vessel wall after that point and will not be spherical. Pressure increase after that point is due to burning of corner gases. The laminar burning speed reported in this thesis is only for smooth and spherical flame before hitting the wall. The assumption made in the current model is that gases within the combustion chamber consist of burned and unburned regions separated through a reaction layer of zero thickness as illustrated in figure 15. The burned gas within the center of the chamber is divided into n number of shells when the number of shells is proportional to combustion duration. For example, when combustion takes long time, number of shells is high and vice versa. The temperatures of burned gases in the shells differ from each other and burned gases are at chemical equilibrium state in each shell at a specific temperature. Unburned gas surrounds the burned gas and the preheat zone ($\delta_{ph}$) separate the unburned gas from the burned gas. Core unburned gas has a uniform temperature. There is a boundary layer ($\delta_{bl}$) that separates the core unburned gases from the vessel wall. Additional assumptions made are that the unburned and burned gases are ideal, unburned gas is frozen in its initial chemical composition, the chamber is under uniform pressure, compression of both the unburned and burned gases is isentropic. The JANAF Tables and STANJAN code [72-73] are then used to obtain the thermodynamic properties of unburned and burned gas.
3.2.1. Assumptions

The following assumptions have been used:

- Negligible Reaction Sheet, \( d_\ell \ll r_\ell \).
- Unburned Gas is Compressed Isentropically.
- Unburned Gas is frozen in its Initial Chemical Composition.
- There are \( n \) number of burned gas shells.
- The Burned Gas Shells are in Chemical Equilibrium and gases in different shells are compressed isentropically, as combustion proceeds.
Energy Transfer to the Vessel: Conduction in Boundary Layer from the Unburned Gas, Conduction from Burned and Unburned gas to electrodes and Radiation from the Burned Gas.

Figure 15: Schematic of different zones and their corresponding temperatures in the thermodynamics model.

3.2.1. Burned Gas Mass Fraction and Temperature

For the spherical flames, the determination of the distribution of temperature of gases within the combustion chamber as well as burned gas mass fractions is done through the measured pressure and using conservation of mass and energy equation as well as the equation for ideal gas.
\[ pv = RT \] \hspace{2cm} (3.1)

In equation 3.1

\[ p = \text{pressure} \]

\[ v = \text{specific volume} \]

\[ R = \text{specific gas constant} = \frac{\bar{R}}{M} = \frac{8.314}{M} \]

\[ M = \text{Molar mass} \]

\[ T = \text{temperature} \]

The equation 3.2 gives the mass conservation

\[ m = m_b + m_u = \rho_b V_b + \rho_u V_u = p_i (V_c - V_e) / RT_i \] \hspace{2cm} (3.2)

In equation 3.2

\[ m = \text{mass of gas within the combustion chamber} \]

\[ m_b = \text{mass of burned gas} \]

\[ m_u = \text{mass of unburned gas} \]

\[ V_c = \text{volume of the combustion chamber} \]

\[ V_e = \text{electrode volume} \]

Subscript i depict initial conditions

Subscripts b denote burned conditions while u denote unburned conditions

\[ \rho = \text{average density} \]

\[ V = \text{volume of the gas} \]

The overall gas volume in combustion chamber is

\[ V_i = V_c - V_e = V_b + V_u \] \hspace{2cm} (3.3)
Equation for energy conservation is

\[ E_i - Q_e - Q_w - Q_r = E_b + E_u \]  \hspace{1cm} (3.4)

\[ E_i = \text{initial energy for unburned gas} \]
\[ Q_w = \text{conduction heat loss to the wall} \]
\[ Q_e = \text{conduction heat loss to the electrodes} \]
\[ Q_r = \text{heat loss due to radiation from the burned gas.} \]

If there is rapid increase in pressure similar to increases occurring in constant volume combustion, the terms that represent compression work on the boundary layer can be neglected. As such, subsequent equations are

\[ Q_e = pV_{eb}/(\gamma_b - 1) = E_{eb} \] \hspace{1cm} (3.5)

\[ Q_w = pV_{wb}/(\gamma_u - 1) = E_{wb} \] \hspace{1cm} (3.6)

Equation 3.7 is used to calculate the radiation energy loss of the burned gases

\[ Q_r = \int_0^i Q_r(t') \, dt' = 4\alpha_p V_b \sigma T_b^4 \] \hspace{1cm} (3.7)

\[ \alpha_p = \text{coefficient for Planck mean absorption} \]
\[ \sigma = \text{Stefan- Boltzmann constant [74-79].} \]
Finally, as it is demonstrated in appendix B, the following equations of volume and energy solved simultaneously.

\[
\int_{0}^{m_b} v_{b\infty} \, dm + (1 - x_b) v_{u\infty} = \frac{V_c - V_e}{m} + \frac{4\pi r_e^2 \delta_{wb} + 2\pi r_e r_b \delta_{eb} + 4\pi r_b^2 \delta_{ph}}{m} \quad \ldots \ldots \quad (3.8)
\]

\[
\int_{0}^{m_b} e_{b\infty} \, dm + (1 - x_b) e_{u\infty} = \frac{E}{m} - \frac{A_{wb}}{m} \int_{0}^{\delta_{wb}} P \, d\delta' - \frac{A_{eb}}{m} \int_{0}^{\delta_{eb}} P \, d\delta' - \frac{Q_r}{m} + \frac{PV_{ph}}{m(\gamma_u - 1)} \quad \ldots \ldots \quad \ldots \ldots \quad (3.9)
\]

Where \( v_i = (V_c - V_e)/m \) and \( e_i = E_i/m \) are the original specific volume as well as the energy in the unburned gas within the chamber.

Equations 3.8 and 3.9 have the following unknowns: \( p, x_b(t) \) and \( T_b(r, t) \)

Given the measured pressure, then there are two equations that can be used to solve for \( x_b(t) \) and \( T_b(r, t) \). Newton Raphson method has been used to solve for \( x_b(t) \) and \( T_b(r, t) \). The mass burning rate, \( \dot{m}_b = m\dot{x}_b \) can be found through numerical differentiation of \( x_b(t) \) [64].

### 3.2.2. Burning Speed

The burning speed can be defined as follows

\[
S_u = \frac{\dot{m}_b}{\rho_u A_b} = \frac{m\dot{x}_b}{\rho_u A_b} \quad \ldots \ldots \quad (3.10)
\]

In equation 3.10, \( A_b \) represents area of sphere having volume equal to that of burned gas. \( \rho_u \) is density of unburned gas which can be calculated from \( P(t) \) and \( T_u(t) \).
\[ A_b = 4\pi r_f^2 - 2\pi r_e^2 \] ................................................................. (3.11)

Where \( r_f \) is the flame radius and \( r_e \) is the radius of extended electrode from spark plugs. Flame radius can be calculated from the following equation:

\[ V_b = (4 / 3)\pi r_f^3 - 2\pi r_e r_f^2 \] ................................................................. (3.12)
4. Results

4.1. Stretch Effects

An important factor to consider in the measurement of the burning speed is the impact of curvature and stretch rate. One should apply the corrections for stretch rate to the calculation of burning speed as suggested in many studies if needed [54, 80-81]. It is important to note that the curvature and stretch rate corrections are most significant when the flame’s radius is small and its thickness is of similar order to that of the radius. The impact of the flame thickness can be ignored when the radius of the flame is larger than 4 centimeters. This condition is attained by the time pressure starts to rise, and this is the starting point for the calculations in this study. Accordingly, the correction will diminish as the flame continues to grow and get thinner.

The variation of flame area over time is the cause of stretch. For spherically expanding flames stretch rate can be defined as:

\[ K = \frac{1}{A} \frac{dA}{dt} = \frac{2}{r_f} \frac{dr_f}{dt} \]  

\[(4.1)\]

\( K \) = stretch rate  
\( A \) = area of flame  
\( r_f \) = flame radius  
\( t \) = time

In order to study stretch effect tests have been made to measure the laminar burning speed for GTL/air for \( \phi = 1 \) at same condition; but two different radii having two different stretch rate.
Two experiments for stoichiometric mixture with two different initial conditions were made. The initial conditions were $P_i = 0.7666 \text{ atm}, T_i = 460 \text{ K}$ and $P_i = 1 \text{ atm}, T_i = 490 \text{ K}$. since these two states are on the same isentrop, having the same entropy most of the unburned gases will be in common. Figure 16 shows temperature and pressures of unburned gas states on log-log plot. As it can be seen the unburned gas states lie on a straight line showing isentropic compression.

Laminar burning speed at $T= 500 \text{ K}$ and $P=1.1 \text{ atm}$ has been calculated using the two experiments. The thermodynamic properties of these two states are the same but the flame radii are different, causing different stretch rate for these two flames. Figure 18 shows the laminar burning speed of these two states having two stretch rate. Flame radius at points A and B are 4.4 cm and 4.1 respectively. as it can be seen, burning speed for the given state is independent of the stretch rate since its flame radius is high. It is concluded for these experiments, flames having radii larger than 4 cm stretch does not have a major effect on burning speed. In this thesis laminar burning speed is reported only for flames having larger radius of 4 cm.
Figure 16: Unburned gas conditions along an isentrop for $\varphi=1$

Figure 17: Unburned gas initial conditions along an isentrop for $\varphi=1$
Figure 18 shows values of burning speed of $T = 500$ K and $P = 1.1$ atm with two different radius having two different stretch rate. As it can be seen the burning speed is independent of stretch rate at their high radius (> 4 cm).

Figure 18: Laminar burning speed versus stretch rate for GTL/air mixture

4.2. Laminar Burning Speeds Results

Laminar burning speed measurement for GTL/air mixture at initial temperature of 490 K, three initial pressures of 0.5, 1, 2 atm and a range of equivalence ratios from 0.7 to 1.2 are presented in this section. A comparison between the present study and other studies in literature and also with simulation will be shown in this section.

Correlations have been developed for laminar burning speeds of GTL/air mixture. A power law correlation has been used to fit to the data over all the equivalence ratios, temperatures and pressures.
\[ S_u = S_{u0} (1 + a(1 - \varphi) + b(1 - \varphi)^2) \left( \frac{T_u}{T_{u0}} \right)^{\alpha_0 + \alpha_1 \varphi} \left( \frac{P}{P_0} \right)^{\beta_0 + \beta_1 \varphi} \] .......................... (4.3)

\[ S_u = \text{laminar burning speed} \]
\[ S_{u0} = \text{laminar burning speed at reference point} \]
\[ T_u = \text{unburned gas temperature in K} \]
\[ T_{u0} = \text{reference temperature} = 490K \]
\[ P = \text{mixture pressure in atm} \]
\[ P_0 = \text{reference pressure} = 1 \text{ atm} \]
\[ S_{u0}, a, b, \alpha_0, \alpha_1, \beta_0 \text{ and } \beta_1 \text{ are fitted constants} \]

The least square fitted parameters are shown in table 3 with R-squared equal to (0.96945). These parameters were fitted over pressure range from 0.5 to 4.3 atm, equivalence ratios from 0.7 to 1.2 and temperature range of 490 K > T > 620 K.

<table>
<thead>
<tr>
<th>( S_{u0} \left( \frac{cm}{s} \right) )</th>
<th>( a )</th>
<th>( b )</th>
<th>( \alpha_0 )</th>
<th>( \alpha_1 )</th>
<th>( \beta_0 )</th>
<th>( \beta_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>85.184</td>
<td>-0.4936</td>
<td>-2.2585</td>
<td>2.1645</td>
<td>-0.0829</td>
<td>-0.3773</td>
<td>0.2192</td>
</tr>
</tbody>
</table>

Table 3: Fitted parameters for GTL/air burning speeds correlation.

Figures 19 to 23 show laminar burning speeds of GTL-air mixtures with initial temperature of 490 K and initial pressures of 0.5, 1.0 and 2.0 atm for different equivalence ratios along isentropes. The fitted values of equation 4.3 are also shown as straight curves in the figures. Based on the burning speed results of those conditions, it was noted that the laminar burning speed is proportional directly to temperature and inversely to pressure. Figure 24 shows laminar burning speeds of GTL-air mixtures with initial temperature of 490 K and initial pressures of 0.5 atm for different equivalence ratios. It is noted that the highest laminar
burning speed is when $\varphi = 1.12$ and the lowest when $\varphi = 0.7$. Figure 25 shows laminar burning speeds of GTL-air mixtures with initial temperature of 490 K and initial pressures of 1.0 atm for different equivalence ratios and it shows the same behavior as the previous condition. Figure 26 shows laminar burning speeds of GTL-air mixtures with initial temperature of 490 K and initial pressures of 2.0 atm for different equivalence ratios. For this condition we did not calculate the laminar burning speed for the rich mixture since they are completely cellular. Figure 27 shows laminar burning speeds of GTL-air flames for different pressures, equivalence ratios and $T = 490$ K. This figure shows that the laminar burning speed is increasing as the pressure decrease and also shows the maximum and the minimum laminar burning speed at $\varphi = 1.12$ and $\varphi = 0.7$ respectively.
Figure 20: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\phi = 0.85$

Figure 21: Laminar burning speeds of GTL-air flames for different pressures $T_i = 490$ K, $\phi = 1.0$
Figure 22: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\phi = 1.12$

Figure 23: Laminar burning speeds of GTL-air flames for different pressures, $T_i = 490$ K, $\phi = 1.2$
Figure 24: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i=490$ K, $P_i=0.5$ atm.

Figure 25: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i=490$ K, $P_i=1.0$ atm.
Figure 26: Laminar burning speeds of GTL-air flames for different equivalence ratios, $T_i = 490$ K, $P_i=2.0$ atm.

Figure 27: Laminar burning speeds of GTL-air flames for different pressures, equivalence ratios and $T_i = 490$ K.
4.3. Comparison

As mentioned in chapter 1, since there is no laminar speed data in the literature for GTL/air mixture at 490 K which is the initial temperature condition that has been considered in this study, laminar burning speeds from this study have been compared with experimental data in the literature for lower temperatures at standard atmospheric pressure for a range of equivalence ratios 0.7-1.2 as shown in Figure 28. The results of this study is higher than the literature values, this is because we operate at higher temperature which is true as the laminar burning speed is directly proportional to temperature. Another comparison with simulation that has been done by my co-worker [82] at the same temperature and pressure is shown in Figure 29-31. The simulation gives a higher results than the experiments.

Figure 28: Comparison of measured laminar burning speeds of GTL-air with other reported values at T= 490 K and P= 1 atm as a function of fuel/air equivalence ratios
Table 29: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, $T=490$ K, $P=1.0$ atm

Figure 30: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, $T=490$ K, $P=0.5$ atm
Figure 31: Comparison of measured laminar burning speeds of GTL-air with simulation results for different equivalence ratios, T=490 K, P=2 atm
5. Summary, Conclusions and Recommendations

Laminar burning speed and flame structure of gas-to-liquid (GTL) fuel has been experimentally measured and analyzed using cylindrical vessel. The dynamic combustion pressure measured from the cylindrical vessel is the input for the burning model to calculate burning speed. The burning model used to calculate the burning speed from the pressure rise includes the radiation losses from burned gas to the wall of the vessel, temperature gradient in preheat zone and energy loss due to electrodes. A code has been written to calculate the burning speed for GTL. NASA polynomial coefficients has been used in the code to calculate the unburned properties while STANJAN was used for the burned gas properties calculation.

Burning speed measurements have been done only for smooth flames with radii larger than 4 cm. Flame structures of all conditions have been studied and the critical conditions at which cell formations occurred were identified by using optics.

Burning speed of GTL/air mixture have been measured using the cylindrical vessel for initial temperature of 490 K and a wide range of pressures and equivalence ratios. Power low correlation for burning speed of GTL/air mixture has been developed that valid in the range of $0.7 < \varphi < 1.2$, $490 K < T < 620 K$, $0.5 \text{ atm} < P < 4.3 \text{ atm}$.

Based on the experiments, it is concluded that the laminar burning speed is proportional directly to temperature and inversely to pressure.

Laminar burning speeds from this study have been compared with experimental data in the literature for lower temperatures at standard atmospheric pressure for a range of equivalence ratios 0.7-1.2. Our results is higher than the literature, this is because we operate at higher temperature which is true as the laminar burning speed is directly proportional to
temperature. Another comparison with simulation results that has been done by my co-worker at the same initial temperature and pressure.

It is recommended that measurement for burning speed of GTL/air to be conducted at initial temperature of 530 K at which the evaporation rate is 100%. By this it can make sure that all species are burned. This will need modifications to the system to handle up to that temperature.

It is also recommended to study the effects of various parameters on the flame stability and conditions that delays instability in flame by adding a diluent. More quantitative data is needed to study wrinkles and cells emerging on flame surface.
6. References


Mechanisms for Practical High Hydrocarbon Fuels, Combustion Science and Technology, 148 (1999), 93-133


26. Rallis C. J. and Garforth A. M., Determination of Laminar Burning Velocity,


32. Egolfopoulos F. N. and Law C. K., Chain Mechanisms in the Overall Reaction Orders in Laminar Flame Propagation, Combustion and Flame, 80 (1990), 7- 16


42. Tseng, L., Ismail, M., and Faeth, G. Laminar Burning Velocities and Markstein Numbers of Hydrocarbon/Air Flames, Combustion and Flame, 95 (1993), 410-426


50. Ryan, T. W., and Lestz, S. S. The Laminar Burning Velocity of Isooctane, n- Heptane,


58. Clarke, A., Stone, R., and Beckwith, P., Measuring the Laminar Burning Velocity of Methane/Diluent/air Mixtures within a Constant-Volume Combustion Bomb in a Micro-


66. Farazan, Parsinejad ., 2005, ” Experimental and theoretical studies on flame propagation and burning speed of JP-8, JP-10 and reformed fuel at high temperatures and pressures”


73. JANAF Thermochemical Tables, Third Edition, edited by American Chemical Institute and American Institute of Physics, 1986

74. Reynolds W. C., Stanford University Report. 1986, Stanford University


76.

77. Francis, NY 2002


83.


86. Guangying, Yu., Private communication
Appendix A: Laminar burning speed code

PROGRAM MAIN
C     DATE: 05/19/2016
C     DONE BY: MOHAMMED SAAD ALSWAT
C     MAIN PROGRAM THAT CALCULATE THE UNBURNED PROPERTIES FROM THE PRESSURE-TIME DATA
C=====================================================================================**
CDeclare the Variable Arrays **
IMPLICIT REAL*8 (A-H, O-Z), INTEGER (I-N)
REAL*8 :: TU(1000),TUSUB(1000),TNOT,PNOT,PRES(2000),UTOT,VTOT,PHI,
T(2000),VU(1000),U(1000),H(1000),TUDUM,S,PI,PP, XF(1000), ALPHA,
CP(10),CV(10),DENSITY_NOT,AMIX(50),PPA,PTOT,PPF,RMIX,W_MIX,WTOT,
PRES (7500), PRES_SM (2000), T_SM (2000), RED_PRES_SM (7500), RED_T_SM (7500),
TOTAL_NUMBER_OF_MOLES, A (10, 10), SUMS, SUMDS, GAMM, GAM_DUM (100),
USUB(1000),VUSUB(1000),CV_MIX,GAMMA(1000),CPMIX(1000),CMIX(1000),
CP_MIX,d,errf,errx,QOUT(1000),VOUT(1000), THERM_COND,PANSWER,
face(10,10),five(10),pi(10),PRES_INTEG(2000),V_B(1000),
COEF_SIG(10,10),COEF_EPS(10,10),M(10),SIGMA(10),A_F(1000),
LAMDA1(10),LAMDA2(10),LAMDA(10),ETA(10),EPS(10),VELOCITY(1000),
OMEGA1 (10), OMEGA2 (10), LAMDA MIX, THERMAL_COND, TIN, VISC, NN (10),
ANSWER, DISPL_THICK (1000), T_INF, P_INF, POWER, BURNING_RATE (2000),
PRES_SUB (1000), T_SUB (1000), T_INF_SUB, P_INF_SUB, extra, x (2),
DELTA T, INTEGVAR (1000), PART1, PART2, TT (1000), FLAME_THICKNESS (2000),
XX, XF (1000), UUB (1000), VVB (1000), enthalpy (1000),
GAMM_PREV (1000), enthal, TB (1000), XB (1000), DDX (1000),
ORDT (1000), R_F (1000), STR (1000), cond_ratio (1000),
TSTAR (1000), DUMMY (1000)
INTEGER I, J, K, Z, NPT
CHARACTER TIME*4, CH7*4, ATOM*8, CONA*4, CONB*4
DOUBLE PRECISION tolf, tolx, enthalp
$U(1000),VU(1000),GAMM_PREV(1000),PP,TB(1000),XB(1000),x(n),
Common /vole of burned gas/VOL_B, /IPAR/ NIWORK, NICMP, NIKNT, NRWORK,
NRKNT, NRTMP, NRA, NRADD, MAXTP, NPC, NCP1, NCP2, NCP2T,
RPAR/ ER2CAL, RU, RUC, T298, NPHASE, NSMS, NWT, NXCON, NKCON, NAMAX,
NX1, NX2, NY1, NY2, NT1, NT2,
NP1, NP2, NV1, NV2, NW1, NW2,
NS1, NS2, NU1, NU2, NH1, NH2,
NC1, NC2, NCDET, NTEST, NPEST
DIMENSION ICKWRK (*), RCKWRK (*), I EQWRK (*), REQWRK (*),
REAC (*), KCON (*), XCON (*)
LOGICAL LPRNT, EQST, LCNTUE
PARAMETER INTEGER NP=10
C=====================================================================================**
** THE VARIABLES **

TNOT=INITIAL TEMPERATURE,  PNOT=INITIAL PRESSURE

TU=UNBURNED GAS TEMPERATURE,  TUDUM=DUMMY UNBURNED GAS TEMPERATURE

TUSUB=UNBURNED GAS TEMPERATURE PASSED TO SUBROUTINE

PRES=PRESSURE AT ANY TIME

NPT=NUMBER OF POINTS,  ALPHA=HYDROGEN RATIO (FRACTION FROM 0 TO 1)

S=ENTROPY OF MIXTURE,  DS=DERIVATIVE OF ENTROPY

T=TIME,  PHI=STOCHIOMETRIC RATIO

A=JANAF COEFFICIENTS,  AMIX=SUM OF PRODUCT OF MOLE FRACTIONS AND A'S

XF=MOLE FRACTION OF SPECIES,  W_MIX=MOLECULAR WEIGHT OF MIXTURE

PPA=PARTIAL PRESSURE OF AIR,

PPF=PARTIAL PRESSURE OF FUEL,  PTOT=TOTAL PRESSURE

RMIX=GAS CONSTANT FOR MIXTURE,  GAMMA=CP/CV (RATIO OF SPECIFIC HEATS)

GAMM=DUMMY SPECIFIC HEAT RATIO TO PASS TO SUBROUTINE

TB=DUMMY TEMPERATURE TO CHECK THE CKINTP SUBROUTINES

VU=SPECIFIC VOLUME OF UNBURNED GAS

U=SPECIFIC ENERGY OF UNBURNED GAS

** INPUT THAT SHOULD BE CHANGED FOR EACH CASE **

** INITIAL TEMPERATURE AND PRESSURE, PHI AND aa **

WRITE (*,*) TNOT, PNOT, PHI

WRITE (*,*) TNOT, PNOT, PHI
** CALCULATIONS FOR THE TOTAL NUMBER OF MOLES **

\[
\text{PHI} [0.32 \text{ C}_8\text{H}_{18} + 0.25 \text{ C}_{10}\text{H}_{22} + 0.43 \text{ C}_{12}\text{H}_{26}] + 15.83 \text{ O}_2 + 59.52 \text{ N}_2 \quad \text{-----> PRODUCT}
\]

!write (*,*) ALPHAN
TOTAL_NUMBER_OF_MOLES = PHI + 75.35
!Write (*,*) TOTAL_NUMBER_OF_MOLES
Read (*,*)
PPD = 0
PPA = PNOT * (75.35) / (TOTAL_NUMBER_OF_MOLES)
PPF = PNOT - (PPA)
!Write (*,*) 'PPA, PPF, PNOT, PPD'
!READ (*,*)

**READING THE PRESSURE-TIME DATA**

!WRITE (*,*) TNOT
PTOT = PNOT

OPEN (unit=1, FILE='DATA_THERM-for-GTL.DAT')

DO 9 I = 1, 5
!READ (1,*) ATOM
WRITE (*,*) ATOM

READ (1,*) (A (I, J), J = 1, 7)
AMIX (J) = 0.0

WRITE (*,*) (A (I, J), J = 1, 7)
9 CONTINUE

** CALCULATING MOLE FRACTION, MOLFR, AND THE AMIX USING THE A (I, J) **

XF (1) = (0.2095 * PPA/PTOT) ! XF (1) = OXYGEN
XF (2) = (0.7905 * PPA/PTOT) ! XF (2) = Nitrogen
XF (3) = (PHI*0.32) / (TOTAL_NUMBER_OF_MOLES) ! XF (3) = iC8H18
XF (4) = (PHI*0.25) / (TOTAL_NUMBER_OF_MOLES) ! XF (4) = nC10H22
XF (5) = (PHI*0.43) / (TOTAL_NUMBER_OF_MOLES) ! XF (5) = nC12H26
C XF (6) = 0 ! XF (6) = Carbon Dioxide

WRITE (*,*) 'MOLEFRACTIONS:'
WRITE (*,*) XF(1), XF(2), XF(3), XF(4), XF(5)
READ (*,*)
** CALCULATING EACH COEFFICIENT FOR MIXTURE **

DO 3 J=1, 7
    DO 2 I=1, 5
        AMIX (J) = XF (I)*A (I, J) + AMIX (J)
    2 CONTINUE

WRITE (*, 100)
100 FORMAT ('AMIX=',)
    WRITE (*,*) AMIX (J)
3 CONTINUE

** MOLECULAR WIGHT OF THE MIXTURE KG/KMOLE OR G/MOLE **

W_MIX = (XF (1)*(2*15.9994)) + (XF (2)*2*14.0067) + (XF (3)*(114.23266)) +
        (XF (4)*(142.28684)) + (XF (5)*(170.34102))

WRITE (*,*) 'W_MIX'
WRITE (*,*) W_MIX
READ (*,*)

** CALCULATING MIXTURE'S R (KJ/KG.K) **

RMIX = 8.314/W_MIX

WRITE (*,*) 'RMIX'
WRITE (*,*) RMIX
READ (*,*)

CLOSE (1)

** DATA REDUCTION **

NPT=0
J = 0
I = 0
OPEN (unit=2, FILE='PressSMOOTH.dat')
READ (2,*) TIME, CH7
Do while (.NOT.EOF (2))
    NPT=NPT+1
    I=I+1
    READ (2,*) RED_T_SM (I), RED_PRES_SM (I)
    Write (*,*) RED_T_SM (I), RED_PRES_SM (I)
END DO
Write (*,*) 'I am here3'
Read (*,*)
DO I = 1, NPT, 3
  J = J + 1
  TUSUB (J) = TNOT
  Press (J) = RED_PRES_SM (I)
  Press (J) = RED_PRES_SM (I)
  Task (J) = RED_T_SM (I)
  T (J) = RED_T_SM (I)
  Write (*,*) press (j), task (j), t (j)
END DO
NPT = J
CLOSE (2)

C======================================================================
C "N IS THE POWER OF THE PRESSURE FIT, THIS HAS TO BE PASSED TO DISPLACEMNT
THICKNESS SUBROUTINE"

Write (*,*) NPT
INF=NPT
WRITE (*,*)'T (INF), PRES (INF)'
WRITE (*,*) T_SM (INF), PRES_SM (INF)
READ (*,*)
  T (INF) = task (in)
  PRES (INF) = press (in)
  P_INF=PRES_SM (INF)
  T_INF=T_SM (INF)

SUMTIME=0.0
SUMPRES=0.0
DO 320 I=2, NPT
  SUMTIME=SUMTIME + (LOG (T_SM (I)/T_SM (INF))*LOG (T_SM (I)/
                      T_SM (INF)))
  WRITE (*,*)'SUMTIME'
  WRITE (*,*) SUMTIME
  SUMPRES=SUMPRES + (LOG ((PRES_SM (I)-PRES_SM (1))/(PRES_SM (INF)-PRES_SM (1)))*LOG (T_SM (I)/T_SM (INF)))
  WRITE (*,*)'SUMPRES'
  WRITE (*,*) SUMPRES
320  CONTINUE

POWER=SUMPRES/SUMTIME
WRITE (*,*)'POWER OF THE FIT'
WRITE (*,*) POWER
READ (*,*)

C======================================================================
C ** CALCULATING THE UNBURNED TEMPERATURE **

DO 4 I=1, NPT
  Write (*,*) 'I am here4'
  S=2.0
  DS=1.0
  IF (I.EQ.1) THEN
    TUDUM=TNOT+0.1
ELSE
    TUDUM = TUSUB (I-1) + 0.1
ENDIF
PI = PRES (I)

C
** CALCULATING THE ENTROPY AND ITS DERIVATIVE **

WRITE (*,*) TUDUM

C
** USING NEWTON-RAPHSON METHOD TO CALCULATE THE UNBURNED GAS TEMPERATURE **

DO WHILE (ABS(S).GT.0.001)
    SUMS = AMIX (1)*LOG (TUDUM/TNOT)
    SUMDS = AMIX (1)/TUDUM

    WRITE (*,*) 'SUMS, SUMDS'
    WRITE (*,*) SUMS, SUMDS

    DO 232 Z = 2, 5
        SUMS = SUMS + (AMIX (Z)*((TUDUM** (Z-1))-(TNOT** (Z-1)))/ (Z-1))
        SUMDS = SUMDS + (AMIX (Z)*(TUDUM** (Z-2)))
    WRITE (*,*) 'SUMS2, SUMDS2'
    WRITE (*,*) SUMS, SUMDS

    CONTINUE

S = RMIX*(SUMS-LOG (PI/PNOT))
DS = RMIX*SUMDS

WRITE (*, 200)
FORMAT ('S, DS, PI')
WRITE (*,*) S, DS, PI

IF (DS.EQ.0.0) THEN
    WRITE (*,*) 'INVALID DERIVETIVE'
    STOP
ELSE
    TUDUM = TUDUM-(S/DS)
    WRITE (*,*) 'TUDUM IN TUN_SUB='
   WRITE (*,*) TUDUM

    WRITE (*,*) 'PRESS (I), TUDUM'
    WRITE (*,*) PRES (I), TUDUM
ENDIF
ENDDO

TUSUB (I) = TUDUM
TUSUB (1) = TNOT

4   CONTINUE

DO 6 K = 1, NPT
TU (K) = TUSUB (K)
WRITE (*, 300)
300 FORMAT ('UNBURNED GAS TEMP')
WRITE (*,*) TU (K), PRES (K), K
C read (*,*)
6 CONTINUE
C===============================================================================
C                     ** CALCULATING THE SPECIFIC ENERGY **
C===============================================================================
DO 212 J=1, NPT
   U (J) = (AMIX (1) + (AMIX (2)*TU (J)/2) +
   ((AMIX (3)/3)*(TU (J)**2)) +
   ((AMIX (4)/4)*(TU (J)**3)) +
   ((AMIX (5)/5)*(TU (J)**4)) +
   (AMIX (6)/TU (J)) * (RMIX * TU (J)) - (RMIX*TU (J))
WRITE (*,*)'U'
WRITE (*,*) U (J), J
212 CONTINUE
C===============================================================================
C                   ** CALCULATES THE SPECIFIC VOLUME **
C===============================================================================
DO 8 I=1, NPT
   VU (I) = RMIX*TU (I)/ (PRES (I)*101.325/14.7)
WRITE (*,*)'VU'
WRITE (*,*) VU (I)
8 CONTINUE
VTOT=VU (1)
WRITE (*,*)'VTOT'
WRITE (*,*) VTOT
UTOT=U (1)
WRITE (*,*)'UTOT'
WRITE (*,*) UTOT
WRITE (*,*)'VOLUME AND ENERGY UNBURNED'
WRITE (*,*) VU (1), U (1)
Read (*,*)
WTOT=1.8533E-03/VU (1)
DENSITY_NOT=1/VU (1)
Write (*,*)'tot, density not'
Write (*,*) tot, density not

C============================================================================================================================
C "BURNED PROPERITES"
C============================================================================================================================
C "CALCULATING GAMMA FOR THE MIXTURE AT ANY POINT"

DO 101 K=1, NPT
   GAMM=0.0
   WRITE (*,*)'K, TU (K)'
   WRITE (*,*) K, TU (K)

   DO 11 I=1, 5
      CP (I) =0.0

   C "CALCULATING C_P"
   DO 12 J=1, 5
      CP(I)=CP(I)+((A(I,J)*((TU(K)**(J-1)))*8.314)
   12     CONTINUE

   C "CALCULATING C_V AND GAMM"

   GAM_DUM (I) =CP (I)/CV (I)
   11    CONTINUE

   CP_MIX = 0.
   CV_MIX = 0.
   GAMM = 0.

   DO 13 I=1, 5

   C "CALCULATING GAMMA AND CP FOR THE MIXTURE"

   CP_MIX = CP_MIX + CP (I) * XF (I)
   CV_MIX = CP_MIX -8.314
   GAMM = CP_MIX/CV_MIX
   13    CONTINUE

   GAMMA (K) =GAMM
   CPMIX (K) = CP_MIX
   WRITE (*,*) CP_MIX
   WRITE (*, 600)
FORMAT ('GAMMA UNBURNED GAS AT EACH POINT')
WRITE (*,*) GAMMA (K), k
C READ (*,*)
C write (*,*) 'I am here at the beginning of error check'
101 CONTINUE

C="CALCULATING THE VISCOSITY AND THERMAL CONDUCTIVITY OF THE MIXTURE"

CALL TRANSPORT (TNOT, CP, XF, VISC, THERM_COND)

C="CALCULATES THE DISPLACEMENT THICKNESS"

ANSWER=0.0
DELTAT=0.0
P_INF_SUB=P_INF/14.7
T_INF_SUB=T_INF/1000.0
DISPL_THICK (1)=0.0
WRITE (*,*)'DENSITY NOT IN SUB., VISC'
WRITE (*,*) DENSITY_NOT, VISC

DO 155 J=1, NPT
PRES_SUB (J)=PRES (J)/14.7
T_SUB (J)=T (J)/1000.0
155 CONTINUE

DO 1 I=2, NPT
J=I-1

DO 255 K=1, J

IF (GAMMA (K).GT.0.0) THEN
PART1= (((PRES_SUB (K)/PRES_SUB (1)) ** ((GAMMA (K)-1)/GAMMA (K))-1.0)**((PRES_SUB (K)/PRES_SUB (1)) ** (1.0/GAMMA (K))))
ELSE
PART1=0.0
ENDIF

IF (T_SUB (K).EQ.0.0) THEN
PART2=(1/ ((T_SUB (I)-T_SUB (K)) + (P_INF_SUB-PRES_SUB (1))*(T_SUB (I)**(POWER+1)))/ ((POWER+1)*PRES_SUB (1)*T_INF_SUB**POWER)))**0.5
ELSE
PART2=(1/ ((T_SUB (I)-T_SUB (K)) + (P_INF_SUB-PRES_SUB (1))**(POWER+1)))/( ((POWER+1)*PRES_SUB (1)*(T_INF_SUB**POWER)))**0.5
ENDIF

INTEGVAR (K)=PART1*PART2
CONTINUE

DELTAT= (T_SUB (I)-T_SUB (I-1))
IF (J.EQ.1) THEN
   CALL INTEG (2, T_SUB, INTEGVAR, ANSWER)
ELSE
   CALL INTEG (J, T_SUB, INTEGVAR, ANSWER)
ENDIF

EXTRA=2.0*(((PRES_SUB (I)/PRES_SUB (1)) ** ((GAMMA (I)-1)/
   GAMMA (I)))-1.0)*((DELTAT*PRES_SUB (1)/PRES_SUB (I)) *
   0.5)
Write (*,*),'extra'
Write (*,*), extra

DISPL_THICK (I) = (extra+ANSWER)*((VISC/ (3.1415*DENSITY_NOT)) **0.5)
WRITE ('I, DISPLACEMENT THICKNESS, EXTRA'
WRITE (*,*), I, DISPL_THICK (I), EXTRA

C READ (*,*)
Quote (I) =0.0
Out (I) =0.0
DO 110 I=2, NPT
   PRES_INTEG (I) =PRES_SM (I)/14.7

C "INTEGRATING THE PRESSURE RESPECT TO DISPLACEMENT THICKNESS"

   CALL INTEG (I, DISPL_THICK, PRES_INTEG, PANSWER)
   WRITE (*,*), PANSWER, WTOT

C "HEAT AND VOLUME OF THE DISPLACEMENT THICKNESS (BOUNDARY LAYER)"

   QOUT (I)=0.072966*PANSWER*101.325/WTOT
   VOUT (I) =0.072966*DISPL_THICK (I)/WTOT
   WRITE ('I, DIPLACE, QOUT, VOUT'
   WRITE (*,*), I, DISPL_THICK (I), QOUT (I), VOUT (I)

110 CONTINUE

CCCCCCCCCCCCCCCCCCCCCCCC
OPEN (56, file='debug-STANJAN.dat')
WRITE (56,890)

890 FORMAT ('NA', 5x, 'L', 6x, 'TF', 15x, 'P', 16x, 'Vb', 15x, 'Hb', 15x,
   'Up', 15x, 'S', 16x, 'Cp', 15x, 'Cv', 15x,
   'W', 16x, 'XX')

CCCCCCCCCCCCCCCCCCCCCCCCCCC
C "CALLING THE STANJAN AND CALCULATING THE BURNED"

XP=0.0
EP=0.0
VP=0.0

213 DO 350 I=2, NPT
C "CALCULATING THE TOTAL VOLUME AND TOTAL ENERGY CONSIDERING THE DISPLACEMENT THICKNESS"

UTOT=U (1)-QOUT (I)
C U (1) =UTOT-QOUT (I)
VU (1) =VTOT+VOUT (I)
C "INITIALIZING THE TOLERANCE AND NUMBER OF TRIALS AND THE NUMBER OF UNKNOWN VARIABLES (BURNED GAS TEMPERATURE NAD MASS FRACTION BURNED)"

NTRIAL=1000
N=2
TOLX=0.0001
TOLF=0.0001
TB_AVE=0.0
IF (I.EQ.2) THEN
   X (1) =0.011
   X (2) =2500.0
ENDIF
C "SOLVE THE TWO EQUATIONS AND TWO UNKNOWNS"

CALL MNEWT(I,U,VU,UTOT,VTOT,EP,VP,PP,GAMM_PREV,TB,NTRIAL,X,XP,
XB, N, TOLX, TOLF, enthalpy)
C "MASS FRACTION BURNED AND BURNED GAS TEMPERATURE ARE RETURNED"

XB (I ) =X (1)
TB (I ) =X (2)
Enthalpy (I ) = enthalpy
C "TOTAL VOLUME OF THE BURNED GAS"

VOL_B=VOL_B*WTOT
C FLAME RADIUS AND AREA OF THE FLAME, SI UNITS
C THE R_F (I ) = (3*VOLUME OF BURNED GAS/4*PI) ^1/3
C VOLUME OF BURNED GAS=WTOT*X (B)*SPECIFIC VOLUME OF BURNED GAS

V_B (I ) =VOL_B*XB (I)
R_F (I ) = (3.0*V_B (I )/ (4.0*3.14159)) ** (1.0/3.0)
A_F (I ) =4*3.14159*(R_F (I ) **2.0)
C WRITE (*,* ) A_F (I ), V_B (I )
C READ (*,* )

pp = PNOT/14.7
CONTINUE

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CLOSE (56)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Write (*,*)
Write (*,*) 'I am here at the beginning of error check!

C "DERIVATIVE OF MASS FRACTION BURNED RESPECT TO TIME"

CALL XDOT (NPT, T, XB, DXDT)

CALL STRETCH (NPT, T, R_F, DRDT, STR)

OPEN (4, FILE='OUTPUTVELOCITY.dat')

DO 360 K=2, NPT

C "CALCULATING THE VELOCITY (M/SEC)"

VELOCIY (K) =WTOT*(DXDT (K)*1.0E3)*VU (K)/A_F (K)
BURNING_RATE (K) = WTOT * DXDT (K)

C "CALCULATING THE FLAME THICKNESS USING RALLIS & GARFORTH"

FLAME_THICKNESS (K) = (4.6 * THERM_COND * VU (K)) / (CPMIX (K) * VELOCITY (K))

Do 919 I = 1, npt
    cond_ratio (I) = -quote (I) / u (I)
919 continue

BURNING_RATE (K) = (WTOT*1.0E3)*(DXDT (K)*1.0E3)/(A_F (K)*1.0E4)

C "STORE DATA INTO DATA FILES"

Write (4,*) R_F (k)*1000, TU (K),
&2000 * ((R_F (k+1)-R_F (k))/ (t (K+1)-t (K)))/(R_F (K)

360 continue
Print *, char (7)
Write (*,*)
Write (*,*)'I survived! :-)'
Pause
ENDPROGRAM MAIN212