

LAMINAR BURNING VELOCITY OF ETHANOL, ACETALDEHYDE AND ETHANOL- ACETALDEHYDE FLAMES

Master's Thesis

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Abstract

The objective of this study is to get new experimental data regarding to the burning velocities of ethanol, acetaldehyde and their mixture which has been performed by the heat flux method. It is known that the heat flux method for determination of laminar burning velocities is an efficient technique since the burning velocity can be determined directly, without applying extrapolations. These laminar burning velocities of the fuel -air mixture were measured by this method at ambient pressure, various temperatures and several ranges of equivalence ratios. The ethanol-acetaldehyde solutions have previously not been studied; therefore there is no literature available for comparison. The results were only compared to modeled burning velocities by Marinov mechanism which has been implemented hereon by CHEMKIN software. There is inconsistency between the modeled and the measured results of ethanol-acetaldehyde mixture while computing the burning velocities. There is limited literature data available for comparison of the present study of acetaldehyde which has been measured at various temperatures and equivalence ratio; whereas, all results of the shape of the curvatures the graphs have shown the same behaviors and the maximum velocity for each temperature under study. Also, the results of acetaldehydes are compared against each other at different temperature and with the modeling results and the previous result. At last, the relationship between the temperature of the unburnt gas and laminar burning velocity has been studied to see their linear behavior. The power exponents have been determined as a function of equivalence ratio. The burning velocity of the ethanol and acetaldehyde show fairly good agreement with previous and modeled results.

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Chapter 1 Introduction

1.1 Background

Today, no one can deny the fact that the world is experiencing global climate change. Increased global warming caused by greenhouse gases is one of the major problems of human being [2]. A lot of research is therefore being carried out in this area to reduce greenhouse gas emissions. One possible way to minimize greenhouse gas emissions could be using biofuels for energy production. Biofuels are organic matter made from plants or biological waste. The carbon dioxide released by the use of biofuel does not increase the amount of greenhouse gases in the atmosphere [1]. All the carbon dioxide released during the use of biofuel takes part in the natural carbon cycle, and it will be absorbed by plants in the vegetative period. Besides, biofuels harm the environment much less than fossil fuels [2]. Biofuels are also renewable sources of energy. Unlike fossil fuels, the amount which are limited and decreases over time with rising oil price, as result bio-fuels are one of the most promising replacements for fossil fuel [3]. Worldwide, there is an increasing interest for substitutes of conventional fuel and much attention is given to the alternative energy sources. Acetaldehyde is a common intermediate of hydrocarbons and biofuels. The study of acetaldehyde combustion is important since it is a fundamental intermediate species formed in the combustion of hydrocarbon and alcohols, especially ethanol, which is being increasingly used as an automobile fuels. The understanding of combustion mechanism of aldehydes is also useful for pollution considerations [4].

Kaiser and co-workers have investigated the combustion of acetaldehyde by using the static reactor at low temperature in 1986 and have validated a detailed chemical reaction mechanism [4]. This mechanism includes O_2 addition reactions, which are unimportant at high temperatures. After four years, the modeling of the combustion of acetaldehyde has been performed by Cavangh et al in 1990 based on the same experimental data. Unfortunately, there is no enough acetaldehyde flame structure data available for comparison with previous modeling results except for Dagaut et al.'s experiments which was performed in 1995 by using a jet-stirred reactor [4]. Combustion acetaldehyde has been only studied in shock tubes at high temperature [4]. These experimental data are important to have a better understanding on the acetaldehyde combustion mechanism at high temperatures.

In light of the aforementioned ideas, this paper will apply the manipulation of the kinetic mechanisms which was proposed by Marinov in 1990; it is made for simulation of ethanol combustion [20]. The Marinov mechanism implemented with CHEMKIN software is used to compare with the experimental results. It is known that the adiabatic laminar burning velocity S_L of a given mixture is a key parameter to study many properties combustion of the given fuel, such as, for understanding of the underlying chemistry, validation of models etc. It is strongly dependent on the stoichiometric ratio, pressure and initial temperature [5].

There are various experimental methods to measure the burning velocity of a liquid fuel such as the heat flux method, the counter flow method, the Bunsen burner method and the closed vessel method. Except the first method, the other methods use extrapolation to find the burning velocity but the heat flux method rather will not use any extrapolation to measure the adiabatic burning velocity which can be determined directly [6]. Therefore, the adiabatic burning velocity of ethanol, acetaldehyde and ethanol-acetaldehyde mixtures will be studied by the heat flux method at various temperatures (298 – 358 K) with several ranges of the equivalent ratios (0.6-1.8). The adiabatic burning velocity for pure ethanol and acetaldehyde have previously been studied, but ethanol-acetaldehyde mixtures have not been studied to the author's knowledge. The experiment measurements of ethanol-acetaldehyde have been compared only with the modeling performed by using Marinov mechanism while the measurements of ethanol and acetaldehyde have been compared with the modeling result and with previous result. The primary objective of this project is to achieve both experimental and numerical studies of the combustion of flame using acetaldehyde as a fuel. The experimental setup has been used to determine laminar burning velocity of premixed flame. This is done by comparing the results of numerical calculation with the experimental data.

1.2 Motivation

Energy is one of the most important factors for the development and the improvement of the standards of human being's life in any country. Today, the world's energy use and supply cannot be seen as sustainable since the way existing technologies are implemented, based on the fact that much of energy supply and use are dependent on fossil fuels [7]. It is known that the need for energy has been increasing at a rate of 3 % on average per year [1]. Thus; renewable energy sources must be expanded in order to maintain the future energy needs in sustainable manner. According to British Petroleum's Energy Outlook 2030, renewables (biofuels, wind, geothermal, and solar) are expected to raise the growth of oil in primary energy. The main energy sources, which include oil, natural gas and coal, are expected to meet 85% of the world's energy demand, while renewable sources will expand significantly [7]. Among many resources of renewable energy, biofuel is a popular renewable energy. Therefore, these days a number of studies are going particularly on biofuels, supporting the research on reducing the cost of squeezing fuel out of biomass, aiming to make it competitive with the fluctuating price of oil. The objective of this project is to see the contribution of acetaldehyde in hydrocarbons and compare its property with other biofuels by studying its adiabatic burning velocity which plays an important role in determining several significant aspects of the combustion process that is measured by the heat flux method.

1.4 Structure

In Chapter 2 basic combustion physics relevant for the study will be described and definition of flame speed, equivalence ratio and laminar premixed flames will be introduced. In Chapter 3 the heat flux method and the experimental setup will be discussed, as well, some important equations will be introduced for calculating the desired unburned gas velocity and the burner plate temperature using thermocouples. In the same chapter also the uncertainties associated with the heat flux method will be explained. In chapter 4 modeling results and its application will be presented. In Chapter 5 experimental data for ethanol, acetaldehyde and ethanol-acetaldehyde mixture burned at various temperatures (298-358 K) and various equivalent ratios (0.6-1.8) will be presented and discussed as well as comparing them with the modeling and with previous results. In the same chapter also the laminar burning velocity of the above fuels has been estimated. In Chapter 6 general conclusions and recommendations will be presented.

Chapter 2 Basic combustion physics

2.1 Ethanol

Ethanol (C₂H₅OH) is a volatile, flammable, clear colorless liquid with a characteristic, agreeable odor and made from feedstock crops such as corn, barley and sugarcane that contain significant amounts of sugar, or materials that can be converted into sugar, such as starch [8]. It is a renewable fuel used to power vehicles and other internal combustion engines. The use of ethanol as a fuel for internal combustion engines, either alone or in combination with other fuels, has been given much attention mostly because of its possible environmental and long-term economic advantages over fossil fuel. It allows the engine to more completely combust the fuel, resulting in fewer emissions. It is produced from plants that control and make use of the energy of the sun. Therefore, it has many advantages as an automotive fuel. There are different type's biofuels; one of them is ethanol. It is a popular alternative fuel to substitute traditional fuel fuels [8]. Ethanol has been shown to have the additional benefit of reducing the formation of NO_x-pollutants in the emission [10].

Table 1: Chemical and physical properties of ethanol [8]

Property	Value
Molecular Formula	C ₂ H ₅ OH
Boiling point	78.37°C
Melting point	-114°C
Density at 20°C	789kg/m ³
Molar Mass	40.06844g/mole
Vapor pressure at 20°C	5.95Kpa
Flash point	13-14°C
Viscosity at 20°C	0.012Pa s

A number of countries are producing and using ethanol in large amounts which are very important to expand ethanol production and use. For example, China, USA, Sweden and Brazil are using large quantities of ethanol as a fuel which addresses global warming concerns, the amount of carbon dioxide produced while burning fossil fuels must be minimized. Ethanol-blended gasoline and ethanol-blended diesel are being considered as feasible alternatives to further lower emission levels [9].

2.2 Acetaldehyde

Acetaldehyde is an organic colorless liquid, volatile at room temperature, having a fruity odor. Both the liquid and the vapors are highly flammable [12]. It is one of the most important saturated aldehydes, occurring widely in nature and being produced on large amount. It occurs naturally in coffee, bread, and ripe fruit and is produced by plants as part of their normal metabolism [11]. It is also produced by oxidation of ethylene. The primary use of acetaldehyde is as an intermediate in the synthesis of other chemical. It is soluble in water, alcohol, ether, benzene, gasoline, and other common organic solvents. It is an intermediate product of higher plant respiration and formed as a product of incomplete combustion such as coffee roasting, burning of tobacco, vehicle exhaust fumes, coal refining and waste processing [12]. It is used as intermediate and will be completely transformed during the syntheses step into another substance. Thus, sometimes acetaldehyde is present in the final product.

Table 2: Chemical and physical properties of acetaldehyde [12]

Property	Value
Molecular Formula	CH ₃ CHO
Molecular weight	44.06g/mole
Melting point	-123.5°C
Boiling point	20.16°C
Density at 18°C	0.783g/ml
Vapor pressure at 20°C	0.97atm
Flash point(closed cup)	-38°C
Solubility in water at 25°C	Infinite
Viscosity at 20°C	13.570Pa s

Acetaldehyde is the first metabolite in the oxidation of ethanol [12]. It is toxic when applied externally for long periods, an irritant, and a probable carcinogen. It is an air pollutant resulting from combustion, such as automotive exhaust, tobacco smoke etc.

2.3 Mechanism of modeling

This section is provided a short discussion on numerical combustion modeling. CHEMKIN software is used for simulating the combustion of a fuel-oxidizer mixture with the Marinov mechanism. The mechanism of acetaldehyde decomposition is an essential part of the acetaldehyde combustion so it is useful to study the decomposition and combustion mechanism of acetaldehyde together [4]. The Marinov mechanism has been developed to

model the ethanol combustion and therefore it is also applicable to study the acetaldehyde reaction, which is an important intermediate species in the ethanol combustion [20]. These calculations are used to compare with the experimental results. The Marinov mechanism has been chosen for modeling of ethanol, acetaldehyde and ethanol-acetaldehyde mixture. Since it contains the detailed kinetic chemical reaction about ethanol, acetaldehyde and their mixture, it ensures a reasonably good modeling of the acetaldehyde flame. These are the reasons help to choose and apply Marinov mechanism in this project.

2.4 Equivalence ratio

The ratio between the numbers of moles in the fuel relative to the number of moles of oxygen in a mixture is called the equivalence ratio. The measurements are usually being done at different equivalence ratios to conclude how the combustion behaves at a shortage or excess of air.

$$\Phi = \frac{\text{fuel-to-oxidizer ratio}}{(\text{fuel-to-oxidizer ratio})_{st}} = \frac{\text{mass of the fuel/mass of oxygen}}{(\text{mass of the fuel/mass of oxygen})_{st}} \quad \dots 2.1$$

$$= \frac{\text{number of mole of the fuel/number of mole of oxygen}}{(\text{number of mole of the fuel/number of mole of oxygen})_{st}} \quad [17]$$

Here, the suffix S_t stands for stoichiometric conditions.

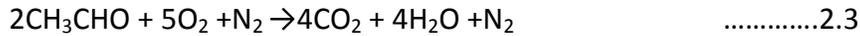
The only products generated in the reaction then are energy, water and carbon dioxide. Theoretically, a complete combustion is achieved when the equivalence ratio equals 1. For $\Phi > 1$ indicates fuel-rich mixtures (excess fuel), and for $\Phi < 1$ indicates fuel-lean mixtures (excess oxidizer). The limits are $\Phi = 0$ for pure oxidizer and $\Phi = \infty$ (infinite) for pure fuel.

2.5 Laminar burning velocity

The burning velocity of a flame is an essential parameter in combustion physics, which is used in various areas such as burner, engines and chemical kinetic validation [6]. The laminar burning velocity is commonly defined as the velocity that a planar flame front travels relative to the unburned gas in a direction normal to the flame surface [13]. A fuel-oxidizer mixture enters the system at the unburnt velocity v_g . A flame front propagates with velocity, S_L , in the unburnt mixture. The flame will remain at a fixed position in space only when the gas velocity v_g equals the adiabatic burning velocity S_L exactly. The adiabatic laminar burning velocity, S_L , is achieved when the velocity of the unburned gas matches that of the flame front, creating a stationary flame [13].

2.6 Laminar premixed flames

There are two types' of flames: premixed flame and non-premixed flame. In this study only focus about premixed flame. A premixed flame of the fuel and the oxidant are mixed before the combustion process takes place. The flames produced in this project are called laminar premixed flames. Because of working with liquid fuels in this project, the fuel-air mixtures are in a gas phase [10]. The overall reaction for acetaldehyde combustion reads



The stoichiometric factor S is defined as the ratio of oxygen and fuel in the overall reaction which is given in equation 2.4. From reaction (2.3), it can be seen that for acetaldehyde $S_{molar} = \frac{5}{2} = 2.5$. The ratio of fuel and oxidizer in a gas mixture is expressed using the equivalence ratio Φ , which is defined in equation 2.1.

$$S_{molar} = \frac{\text{number of mole of oxygen}}{\text{number of mole of fuel}} \quad \dots\dots\dots 2.4$$

Chapter 3 The Heat flux method

3.1 Introduction

The heat flux method is one of the techniques used to determine the adiabatic burning velocity of gaseous mixtures of fuel-oxidizer at ambient pressure and various temperatures [5]. This method does not need any extrapolation due to neither stretch nor heat loss effect and producing a flame, which can be investigated in a laboratory. The perforated burner plate is a core instrument of the setup, which is made of on a brass plate of 2 mm thickness, with hexagonal perforation pattern of small holes having a diameter of 5mm, where a flame is stabilized was introduced by Van Maaren in 1993. This method is based on measuring a temperature distribution which corresponds to the heat loss of the flame to the burner and the heat gain of the unburned gas as it passes through the burner plate. The temperature distribution can be measured by means of small thermocouples attached to the burner plate, and represents the extent in which the flame is stabilized on the burner, because this temperature distribution actually corresponds to the heat loss. This chapter is to explain all the aspects of the heat flux setup resulting in an accurate, reliable and reproducible measurement procedure. In section 3.2 the basic principles of the heat flux method are briefly discussed. The experimental setup will be sketched in section 3.3 followed by a typical measurement. Finally an analysis of the expected uncertainties in the experiment will be presented.

3.2 Principle.

The heat flux method is already examined in the former study to determine the adiabatic burning velocity for various hydrocarbons. To determine this velocity we have used this method which is based on the net heat loss from the flame to the burner and adjusting the gas velocity until situation is reached when no net heat loss is observed as a result of the flame adiabatic state. The generated flame is stretch free since the burner plate will compensate for the heat loss and no extrapolation to zero stretch or heat loss. By varying the gas velocity until a constant temperature distribution is achieved the laminar flame speed can be obtained directly. This will allow for a direct measurement of the laminar flame speed. The heat flux burner is given in the figure 3.1 which shows the heat balance [14] as seen in the figure 3.1.

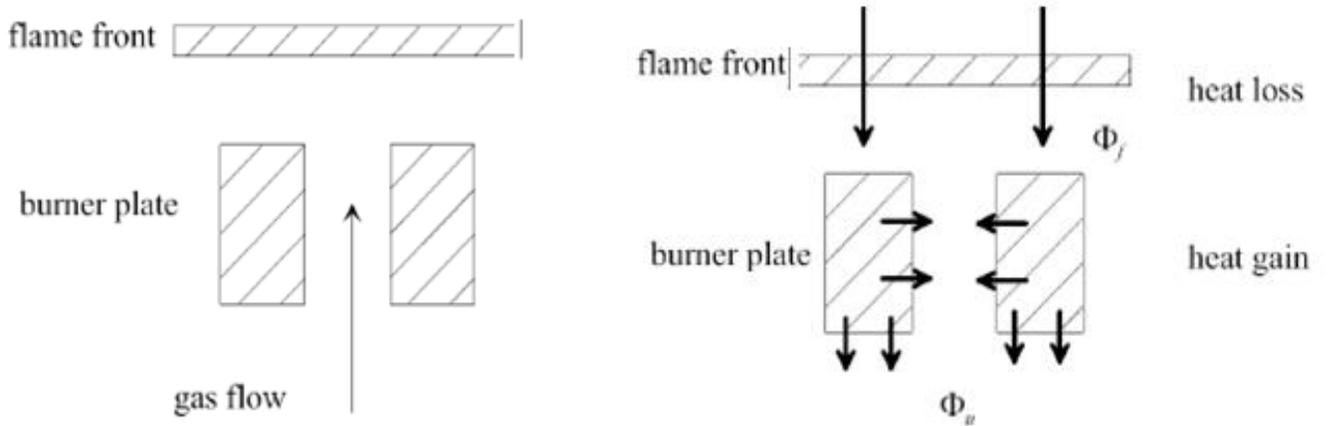


Figure 3.1: Left: The flow of gas in the burner plate, Right: The flow Heat in the burner plate [14].

The principle based on thermodynamics to show the flow of heat. The flame front and burner plate are shown in this figure. The left side presents the flow direction of the gas mixture and the right hand side shows the flow of heat from the flame to the plate and from the plate to the gas mixture. The total heat loss from the flame to the burner is denoted by Φ_f and the total heat gain from burner plate to the unburnt gas is also denoted by Φ_u in the figure. The net heat exchange is the difference between energy gain and energy loss ($\Phi_u - \Phi_f$). It is possible to measure the heat difference, which is a paramount parameter for the temperature profile on the plate [15]. When the net heat exchange is equal to zero, there is no heat exchange between the flame and the burner plate and by definition the flame is in adiabatic state.

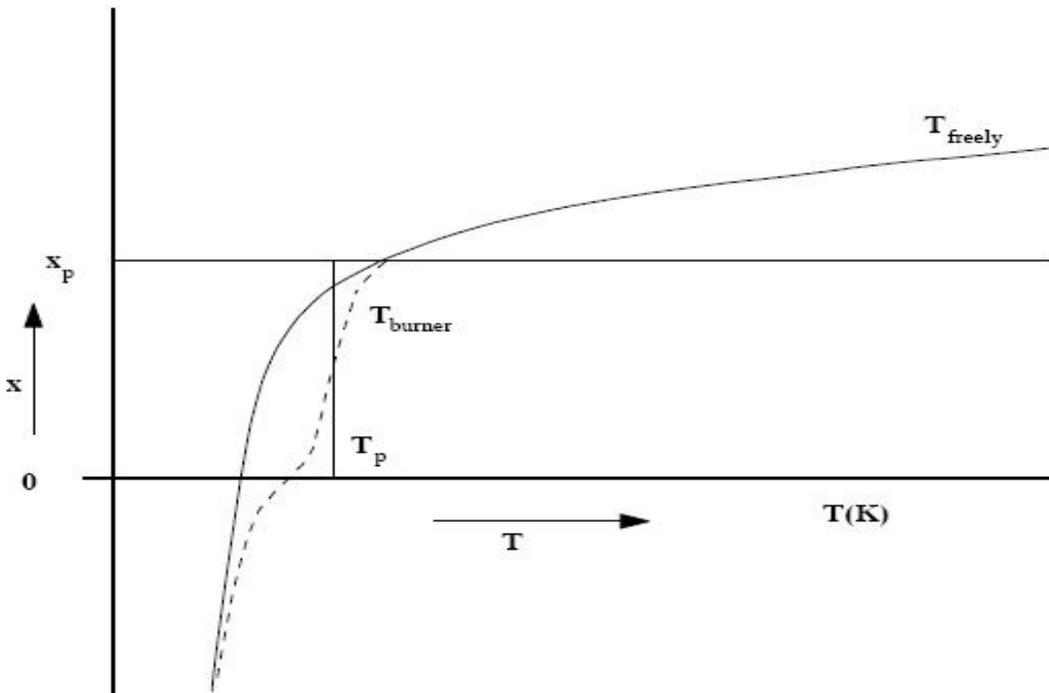


Figure 3.2: Temperature profile of a free and stabilized flame of the burner plate [15].

The temperature profile of a freely propagating flame (T_{freely}) has been compared with the temperature profile of the stabilized flame of the burner plate (T_{burner}) which is given in figure 3.2. In the graph the interval between 0 to x_p shows the thickness of the burner plate in which the straight line T_p is the temperature profile of the burner plate. The temperature distribution of the burner plate corresponds to the net heat loss of the flame to the burner. By varying the velocity of the unburned gas until a constant temperature distribution is reached the adiabatic state can be found [13]. The constant temperature distribution represents zero heat loss in a stretch free flame and no extrapolation is needed.

3.3 Experimental setup

The experimental setup of the heat flux method to be used in this project can be seen in figure 3.3. The core instrument of the setup is the burner used to measure the burning velocity. This is done by measuring the temperature profile of the burner plate through radially spaced thermocouples [13]. The main equipment of the experimental setup of the liquid fuels is given below in table 3. The setup and its components will be discussed in the next section. The fuel is used to measure the adiabatic burning velocity is stored in the fuel tank. The tank is pressurized with argon to protect the fuel from any moisture contamination [6]. To examine a premixed laminar flow, it is required to have a combined supply of fuel and oxidizer in a constant flow. This implies the liquid has to be evaporated after which the vapor is added in a constant stream.

Table 3: Main part of the setup [13]

components	function	Manufacturer
Perforated plate Burner	Create stabilized flame	Bosschaart [6]
Evaporator (CEM)	Evaporate liquid flow	Bronkhorst High-Tech
Cori – Flow	Liquid flow control	Bronkhorst High-Tech
MFCs	Gas flow control	Bronkhorst High-Tech
E7210	Interface for CEM, Cori-Flow and MFCs	Bronkhorst High-Tech
Fuel reservoir	Liquid fuel reservoir	Eindhoven University of Technology
Thermostat baths	Temperature control of heating and cooling jacket	VWR
NI 9162 USB Module	Interface between	National instrument.

	thermocouples and PC	
PC (including Lab view program)	Processing data obtained from thermocouples	Lund University of Technology

The two separate flows of air and fuel respectively enter the CEM at opposite sides and exit at the bottom being a gaseous premixed flow. To provide the CEM with the required liquid flow, a fuel tank in combination with a mass flow meter (Cori-Flow) is used. By use of the Cori-Flow, accurate measuring of this flow rate is possible. The CEM on its turn controls the flow rate by the use of feedback from the Cori-Flow, which in turn is regulated by the interface at the requested set-point. The airflow is controlled by two mass flow controllers (MFCs). The first MFC provides a certain amount of carrier gas for the CEM and a second MFC provides an additional airflow after the evaporator in order to acquire the requested mixture composition [15].

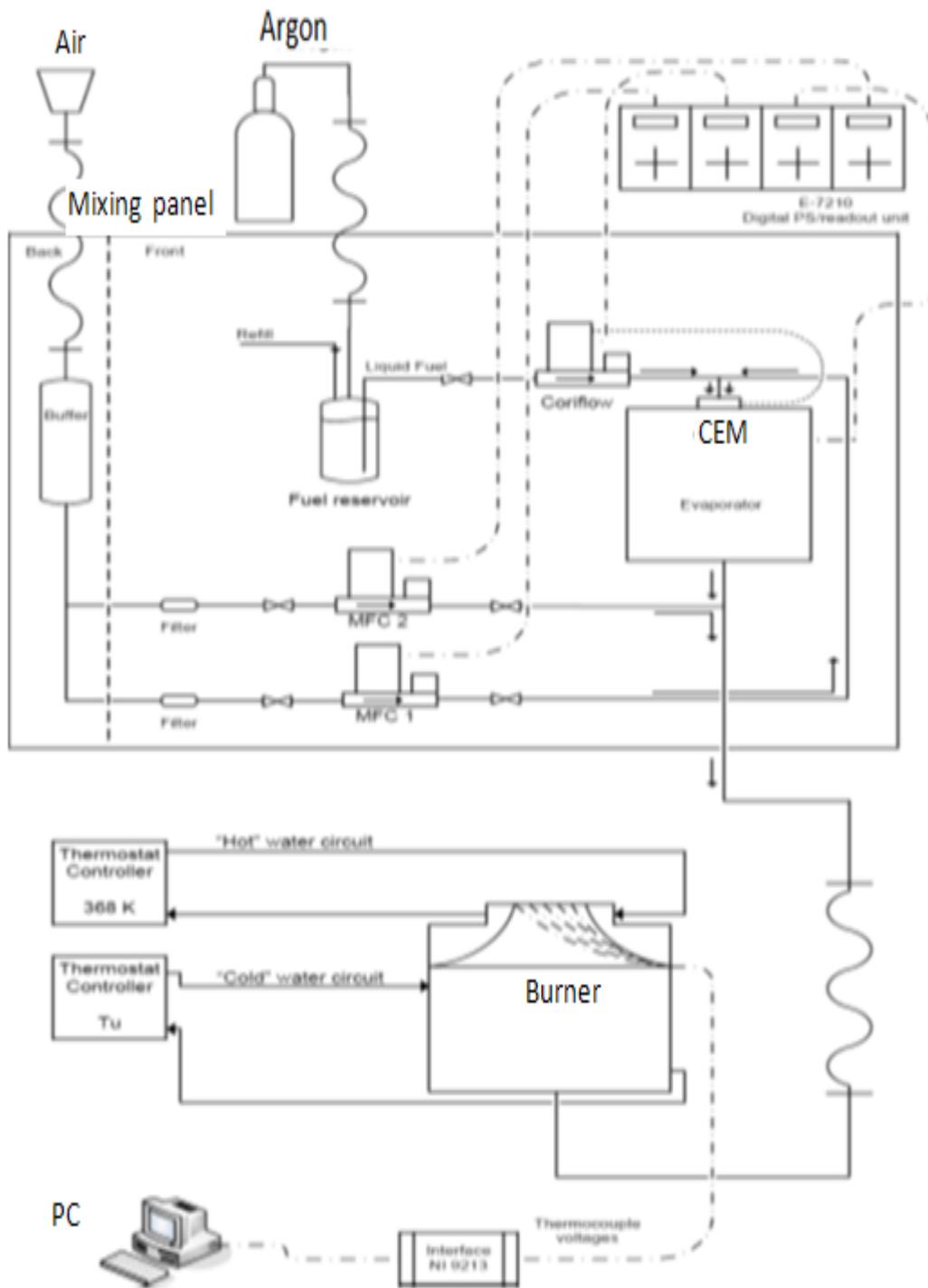


Figure 3.3: Schematic representation of the experimental heat flux setup for liquid fuels [13].

3.4.1 The Burner

The burner given in figure 3.4 consists of a plenum chamber, burner head and burner plate with thermocouples attached and each of its parts will be discussed in the following subsection.

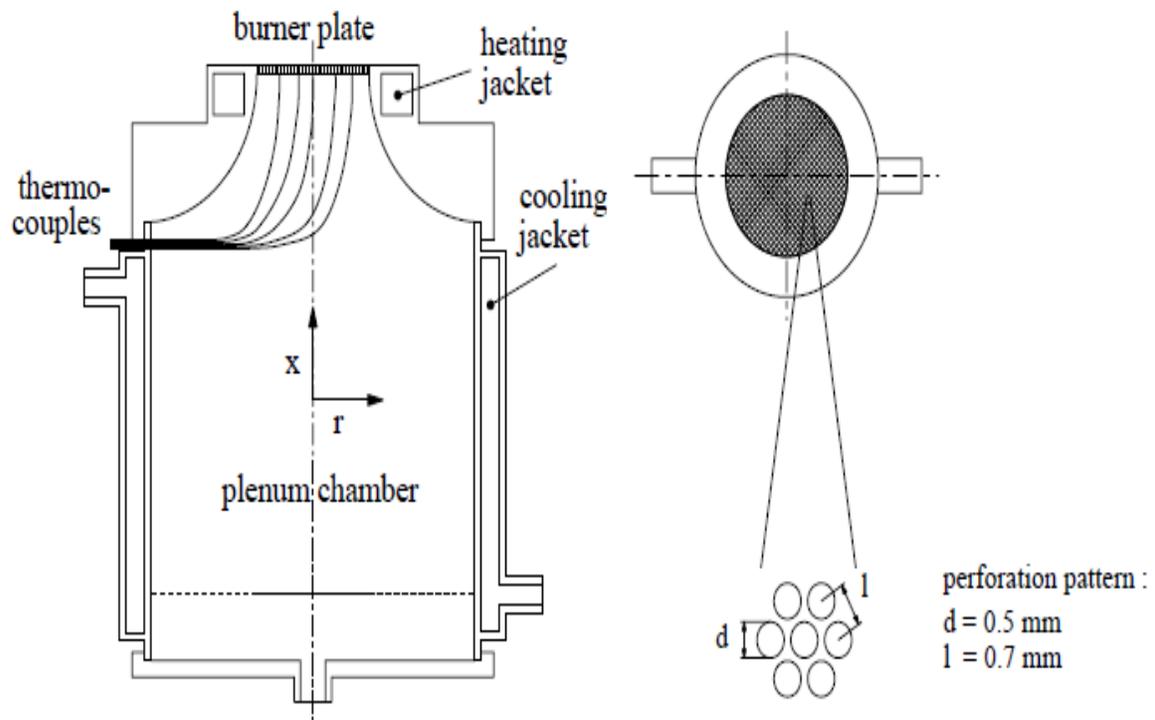


Figure 3.4: Left: The heat flux burner. Right: The perforated burner plate [6].

1 Plenum chamber

The use of the plenum chamber is just to create a uniform flow at the outlet where the burner plate is placed [6]. The temperature of the plenum chamber is controlled by the cooling jacket at required temperature and the temperature of the unburnt gas mixture equals the temperature of the burner chamber [10].

2 Burner head

The schematic overview of the burner head is given in figure 3.5. The burner head has a heating jacket supplied with water from a thermostatic water bath to keep the temperature of the burner plate constant. During the experiments the temperature of the heating jacket was fixed at 368 K [6]. The thermostat baths are used to keep the temperature difference between burner head and burner chamber. There is also a ceramic ring to separate them and to keep at different temperatures.

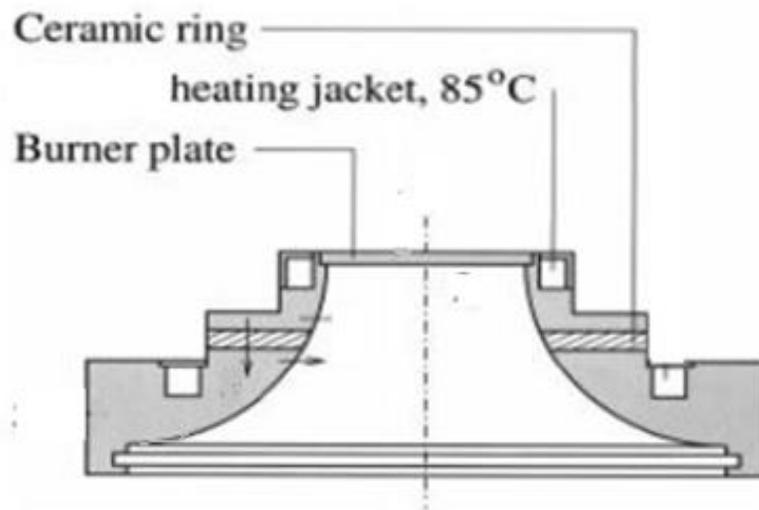


Figure 3.5: A schematic overview of the burner head. [13]

3 Burner plate

The burner plate is made of a brass plate 2 mm thick and 30 mm in diameter, perforated with a hexagonal pattern of small holes with typical diameter 0.5 mm and pitch distance 0.7 mm as shown in figure 3.4. The temperature distribution of the burner plate is measured using the series of thermocouples as shown in figure 3.4 [10].

3.4.2 Thermocouples

The thermocouples have a diameter of 0.31 mm and their function is to determine the temperature distribution of the burner plate. They are placed directly in the holes of the burner plate. The principle is based on placing eight copper wires in the measurement holes of the burner plate [6]. The temperature distribution on the burner plate is measured by thermocouples distributed at different radial places. In the present set up, the thermocouples are inserted at different radial positions on the burner plate i.e. $R = [0, 2.1, 4.2, 6.3, 6.3, 8.4, 10.5, 12.6]$ in the burner plate but the thermocouple was broken at the radial position of 8.4mm.

3.4.3 Controlled evaporator mixer (CEM)

The air and fuel flow is controlled by instruments provided by CEM [13]. In order to get a final gaseous mixture, there should be two separate flows: air flow and liquid flow. Their product gas mixture is then entering to the burner. This can be achieved by applying the concept of evaporation. To get the amount of required flow of fuel towards the CEM, a carrier gas (air in this project) is used. This flow is pressurized by the use of Argon injection into the closed fuel tank. When the fuel enters a CEM with in the small orifice, it will encounter carrier gas that will change the fuel into small droplets. The mixing process can be controlled precisely and generates an accurate mixture composition which is made of liquid droplets and carrier gas. After the mixing process, the mixture is externally heated by a metal spiral, which vaporizes the droplets. The CEM can be heated up to the temperature of 368 K and to avoid the condensation of the fuel the partial pressure of the liquid must be lower than the vapor pressure at the present temperature [17].

3.4.4 Mass flow controller (MFC)

The air used for the heat flux setup is clean and dried air in gas bottle [13]. To get the desired equivalence ratio the mass flow of fuel and air must be investigated. The air flow exiting the buffering vessel is divided into two separate channels, one channel MFC1 supplies the CEM with the required carrier gas and the second channel MFC2 is attached after the CEM output channel, which regulates the amount of additional air needed to get the required gas mixture composition [17]. For the liquid fuel the mass flow can be measured by a Cori-flow (MFC77). The fuel is transported to the evaporator by air from MFC1 to obtain the desired equivalence ratio [13].

3.4.5 NI 9213 USB Module

It is used as an interface connection between user and all components of the setup as shown in figure 3.3. The parameters related to laminar burning velocity calculations can be set manually in the Lab view program to control MFC's of the required flow and to ensure correct flow calculations carried out.

3.5 Laminar burning velocity determination

In this section is presented how the laminar adiabatic burning velocity, S_L is determined from the temperature measured by the thermocouple in the burner plate. The temperature profile as a function of the radius of the burner plate can be described by a second order polynomial of the form and given in equation 3.5.

$$T_p(r) = T_{center} - \frac{q}{4\lambda h} r^2 \quad \dots\dots\dots 3.5$$

Here, λ is the burner plate thermal conductivity, h is the burner plate thickness, T_{center} is the temperature in the center of the burner plate, and q is the net heat transfer from the gas to the burner plate. It is also possible rewrite equation 3.5 in terms α –coefficient and is given in equation 3.6.

$$T_p(r) = T_{center} + \alpha r^2 \quad \dots\dots\dots 3.6$$

Where α , the parabolic coefficient, can be written as

$$\alpha = - \frac{q}{4\lambda h}$$

To determine the adiabatic burning velocity, S_L the following idea has to be used in which the velocity where the burner plate's temperature profile approximately is flat, and needs to be found. A flat temperature profile occurs when the parabolic coefficient (α) of temperature fit equals zero. In figure 3.7 the temperature fits have been plotted as a function of their corresponding radial position of the thermocouples. Experiments are generally done for four different unburned gas velocities for each equivalence ratio and for the given temperature of the fuel.

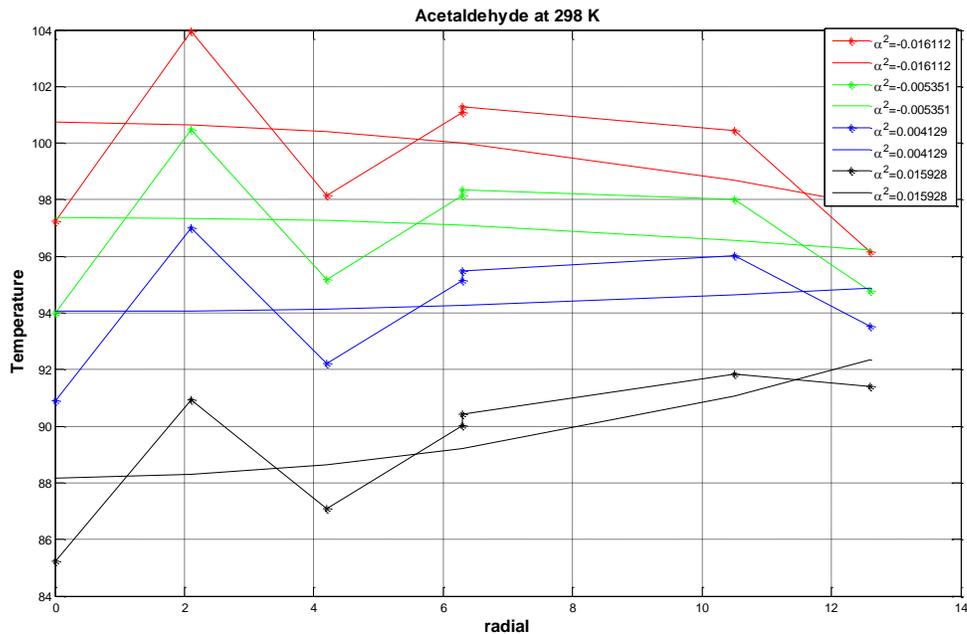


Figure 3.7: The temperature profiles in the burner plate of a stabilized acetaldehyde/air flame at $\Phi=0.9$.

As seen in the figure 3.7 the thermocouple at radial position on 8.4 mm was broken so the reading of the temperature at this point was not correct. The relation between the velocity of the unburned gas mixture and the parabolic coefficient is linear near the adiabatic burning velocity, this is clearly see in figure 3.8. In this case, a lean flame, $\Phi = 0.7$ was used and the adiabatic velocity has been determined to be 19.83 cm/s as seen in figure 3.8 which can be determined by applying interpolation to the obtained data where the parabolic coefficient is equal to zero. When the velocity of the unburned mixture is lower than the adiabatic burning velocity the parabolic coefficient will have negative value and it will have a positive value when the unburned mixture velocity is higher than the adiabatic burning velocity.

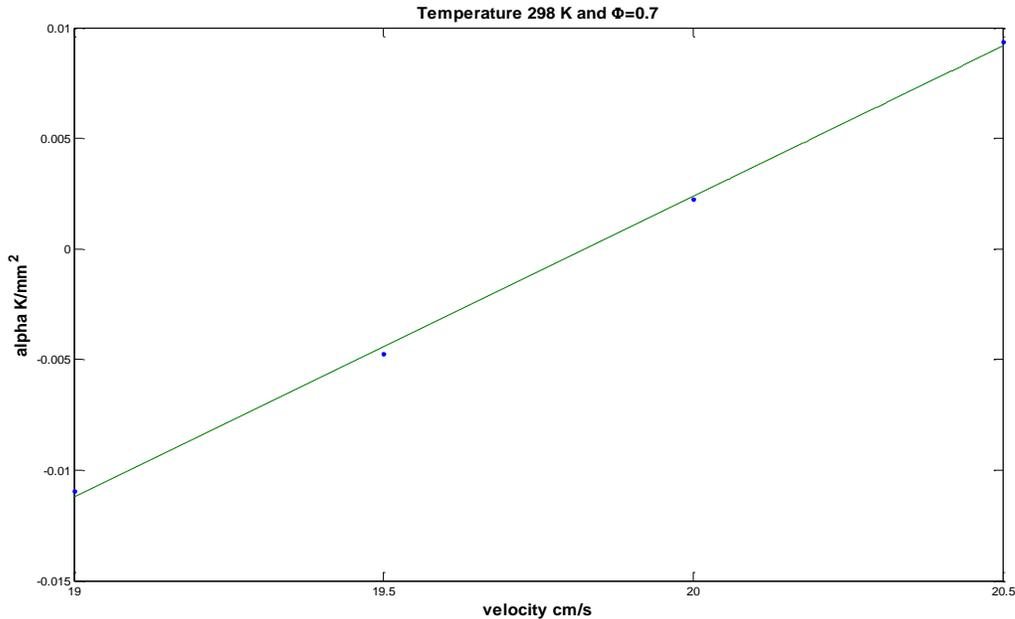


Figure 3.8: The flame speed is determined by calculating the gas speed at which α is zero. In this case for $\Phi = 0.7$, S_L is determined to be 19.83 cm/s.

3.6 Sources of errors

In this section is discussed some of the uncertainties affecting the measurements and the results. The uncertainties are estimated while measuring the laminar burning velocity S_L for the corresponding equivalence ratio. It is obviously true that there are errors; therefore these errors should be analyzed. The analyses of the errors are carried out mainly based on the most important uncertainties which occur during the experiments. The following components of the heat flux method will contribute to the uncertainties of the adiabatic burning velocity during measurement:

- The first type of uncertainty can occur due to the imperfect thermocouple placement on the burner plate.

- The second type of error is due to mass flow, the uncertainty of this will have the largest effect on the laminar flame speed [15]. According to the inaccuracies is given by Bronkhorst in table 4.

- The third type of error is due to the controlled evaporator mixer (CEM); this can affect the flame speed. In 2011 Konnov evaluated that the temperature of the CEM will affect insignificant the flame speed [15].

-The fourth type of error is due to fuel purity; those are of hygroscopic nature the acetaldehyde when the fuel tank is filled with fuel [17].

3.7 Error calculation

The reproducibility test of the results of the experiments on acetaldehyde has been carried out with five temperatures: 298, 318, 338, 348 and 338 K. The burning velocities determined for ethanol-acetaldehyde will be affected by the same uncertainties as acetaldehyde and here also errors being associated with the preparation of the solutions. As discussed in section 3.6 the following component or features of the heat flux method will contribute the most to the uncertainties of the flame speed; thermocouples, controlled evaporator mixer, mass flow controllers and the calibration of the piston meter. The errors are summarized in table 4. For example, there are error bars in figure 5.5 (see chapter 5) associated with the experimental data; these are based on uncertainties of the MFCs and scattering of the thermocouples. The errors are calculated by using the following equations 3.1-3.4.

$$\Delta S_L = \sqrt{\frac{\Delta S_{Lqori} + \Delta S_{Lair} + \Delta S_{Lpiston}}{A}} \quad [\text{m/s}] \quad \dots\dots\dots 3.1$$

Where A (m²) is the area of the burner, $\Delta S_{Lqori} = (\text{fuel} \cdot 0.002)^2$; $\Delta S_{Lpiston} = (\text{Air} \cdot 0.01)^2$; $\Delta S_{Lair} = (0.005 \cdot \text{Air} + 0.001 \cdot \text{Air}_{\text{max}})^2$;

$$\text{Error}_{\alpha} = (\text{STD}(\alpha) / S) / 100; [\text{m/s}] \quad \dots\dots\dots 3.2$$

Where, STD (alpha) is the standard deviation of the linear fit and S is the sensitivity. As seen in figure 3.8, the sensitivity is the slope of the graph which is the ratio alpha to velocity.

The total error due to air flow, fuel flow and piston meter is,

$$S_L = \sqrt{(\Delta S_L)^2 + (\text{Error}_{\alpha})^2} \quad [\text{m/s}] \quad \dots\dots\dots 3.3$$

Where ΔS_L is the error due to MFC flow, Error_{α} is the error due to the thermocouple scattering.

The uncertainty of the equivalence ratio is due to the errors of the MFCs and those that arise during preparation of the solutions. The error is calculated by using equations 3.4.

$$\text{Error}_{\phi} = \phi \cdot (\Phi_{\text{fuel}} + \Phi_{\text{air}} + \Phi_{\text{piston}}) \quad \dots\dots\dots 3.4$$

Where, $\Phi_{\text{fuel}} = (\text{fuel} \cdot 0.001) / \text{fuel}$, $\Phi_{\text{air}} = ((0.005 \cdot \text{Air} + 0.001 \cdot \text{Air}_{\text{max}}) / \text{Air})$ and

$$\Phi_{\text{piston}} = (\text{Air} \cdot 0.01) / \text{Air}$$

Table 4: Summary of the flow of the fluid and Error estimation

Instrument	Fluid	Maximum Capacity of flow of the fluid	uncertainty
MFC1	Air	5 g/min	0.8% of set point, including 0.2% deviation of maximum flow
MFC2	Air	30g/min	0.8% of set point, including 0.2% deviation of maximum flow
MFC77	Liquid	200g/hr.	0.2 % deviation of set point
Controlled evaporator mixer (CEM)	Air	10 l/min	Only affect the burning velocity by 0.05cm/se.

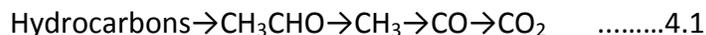
Chapter 4 Chemical kinetics

4.1 Introduction

Chemical reactions occur when molecules of one atom react with molecules of another atom and, for some of these collisions, as a result one or more new molecules will be created. In the chemical reaction the atoms of reacting molecules are rearranged in the new molecules. To achieve this, the reacting molecules must have sufficient kinetic energy so that their chemical bonds can be broken during the impact and other bonds can be formed. As the energy of these bonds depends on the nature of the atoms and on geometrical structure, the energy content of the products of the collision may be different from the energy content of the colliding molecules. This is the basis for heat being released or absorbed in chemical reactions. During these chemical reactions, the overall reactions will consist of hundreds or thousands of such elementary reactions and many species and radicals appear. The series of elementary reactions that comprises the overall reaction process is called a reaction mechanism or a detailed chemical mechanism [21].

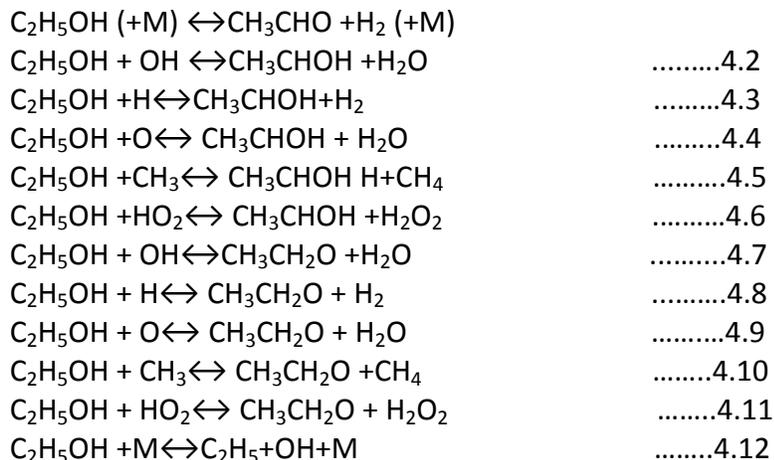
4.2 Combustion chemistry

Combustion is the result of exothermic chemical reactions carried out between a fuel and an oxidant together with the production of heat and conversion of chemical species. The release of heat can produce light in the form of either a flame or glowing [17]. During the burning of a fuel also a few hundred reactions between various compounds have been involved. As discussed in Section 2.2, acetaldehyde is one of the main products in ethanol combustion. Acetaldehyde is a fundamental intermediate species formed while alcohols (especially ethanol) and hydrocarbons burn [20]. It can decompose or react with several different components creating highly reactive species and others products. This all reaction helps to have a good understanding about its chemical reaction scheme. These species can decompose or react with H and OH to generate carbon monoxide, CO, that in turn is transformed into carbon dioxide, CO₂. Much effort has been made by Won et al. in 1995 to investigate the acetaldehyde oxidation in a shock-tube [4]. They obtain a good predication of their experimental results by using a reaction scheme including 110 elementary reactions of 34 species [19]. The initial molecules of a hydrocarbon fuel react with air to yield a variety of reaction intermediates, which then undergo chemical transformations, and finally give the final products, i.e. carbon dioxide (CO₂) and water (H₂O). For the combustion reaction of hydrocarbon the following reaction occurs (4.1).

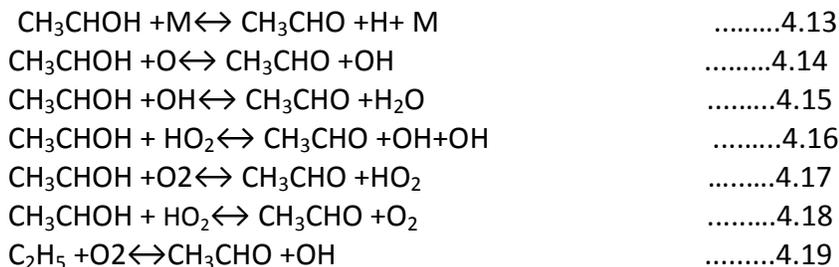


The oxidation of alcohols in flames starts with H-abstraction by H, O and OH. For instance, ethanol oxidation in flames, it first undergoes the H-abstraction reaction. According to ethanol

kinetics the main reactions are involving acetaldehyde production and the combustion process develops according to the chain mechanism of radicals; the steps of the reactions are given in 4.2-4.12 and, resulting in the production of the CH_2CHOH , $\text{CH}_3\text{CH}_2\text{O}$ radicals, or the ethyl radical, C_2H_5 [20].



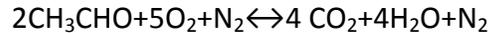
From the above chemical reactions such as CH_3CHOH , $\text{CH}_3\text{CH}_2\text{O}$ and C_2H_5 radicals can undergo either dissociation or hydrogen-abstraction to yield acetaldehyde because they are not very stable as result they react rapidly, as shown in equation, (4.13-4.19) [20].



At the end, acetaldehyde reacts with H, O, and OH producing the CH_3CO radical, followed by its unimolecular decomposition, leading to CH_3 , and CO . From the above explanation it is clear that the ethanol reaction mechanism will lead to chain branching reactions and hydrogen production thus increasing the flame speed [20].

4.3 Modeling

Nowadays, chemical kinetic mechanisms have become an essential instrument to the analysis of combustion systems. The mathematical expression of the problem of chemically reactive flow systems are expressed by the equations of conservation of momentum, mass energy, and each chemical species, together with equations of state and other thermodynamic relationships [19]. Chemical kinetics provides as well the coupling between different chemical species concentration and with the energy equations through the heat of reaction [21]. In many combustion studies the kinetics terms are important to determine the characteristics space and time scales over which equations must be solved [19]. Detailed chemical kinetic models can be used also to predict and analyze the formation physical processes such as flame speed [20]. The mechanisms within a system are consisting of a number of elementary chemical reactions with their rate coefficients determined by fundamental kinetic experiments or theoretical treatment. These mechanisms are the main feature of chemical kinetic models and are developed as response to and validated by a set of experimental measurements. The combustion of acetaldehyde in air is given below with the overall reaction.



This reaction is proceeding, as is well known, through a large number of elementary steps. Besides the experimental validation, the numerical modeling of the adiabatic burning velocities of the acetaldehyde is the main interest in this project. Modeling computations were performed by using the CHEMKIN software and their detailed chemical mechanism, implemented with the Marinov mechanism. The CHEMKIN software can be used to calculate burning velocities of premixed flames, implemented with a proper mechanism and the correct settings thus to determine the flame speed. The following parameters were included: transport properties, were used with multi-component diffusion and thermal diffusion options enabled. Adaptive mesh parameters were GRAD = 0.03 and CURV = 0.05. It is known that these two parameters depend on each other. The total number of grid points was typically 250 – 400. At the end, the modeling results have been compared with experimental results which are found by using the heat flux method.

Chapter 5 Results and Discussion

5.1 Introduction

In this chapter the results of the experimental measurements and numerical calculations are presented and discussed. The heat flux method, as described in chapter 3, has been used to determine the laminar flame speed of ethanol, acetaldehyde and for different percentage concentrations of ethanol-acetaldehyde mixtures. The measurements have been carried out for variable unburnt gas mixture temperatures which are from 298 K to 358 K and the equivalence ratio is varied from 0.7 to 1.8 at 1 atm. The acetaldehyde burning velocity has been repeated four times for each temperature and the ethanol- acetaldehyde mixture has been performed twice for each temperature and a good correlation can be found. It is known that the accuracy of the acetaldehyde burning velocity depends on errors associated with the heat flux setup and impurity of the fuel. In order to validate the experimental results, comparison is made with the previous available data and the modeling results that have been carried out here.

5.2 Laminar burning velocity of pure ethanol at different temperature

In this section are discussed the modeling results of the pure ethanol burning velocities which have been calculated using the Marinov mechanism. These calculations have been used to compare both qualitative and quantitatively results with the experimental results measured previously by various researchers. The previous measurements on the laminar burning velocity of ethanol have been performed by several groups among them Konnov et al. (2011), [22], Lipizig et al. (2011), [18] and Liao et al, [23]. The previous measurements of Konnov et al. (2011) and Lipizig et al. (2011) have been done using the heat flux method whereas the measurement of Liao et al. has been measured using the combustion bomb method. Generally, all these experimental results were achieved three temperatures at 298,318 and 328 K. Almost all the experimental results showed a good agreement with the modeled data results. The results are given in figures 5.1-5.3 below and compared to each other. The highest experimentally determined flame speed is at equivalence ratio 1.1 at 44.29, 44.5 and 49 cm/s at 298, 318 and 328 K, respectively. The results can be compared to the modeled velocities at the corresponding equivalence ratio and temperature 41.6, 44.5 and 47.5cm/s. The vertical error bars of the experimental results arise mainly due to the uncertainty of thermocouples and gas flow control. Good agreements were obtained in its comparison with the literature data.

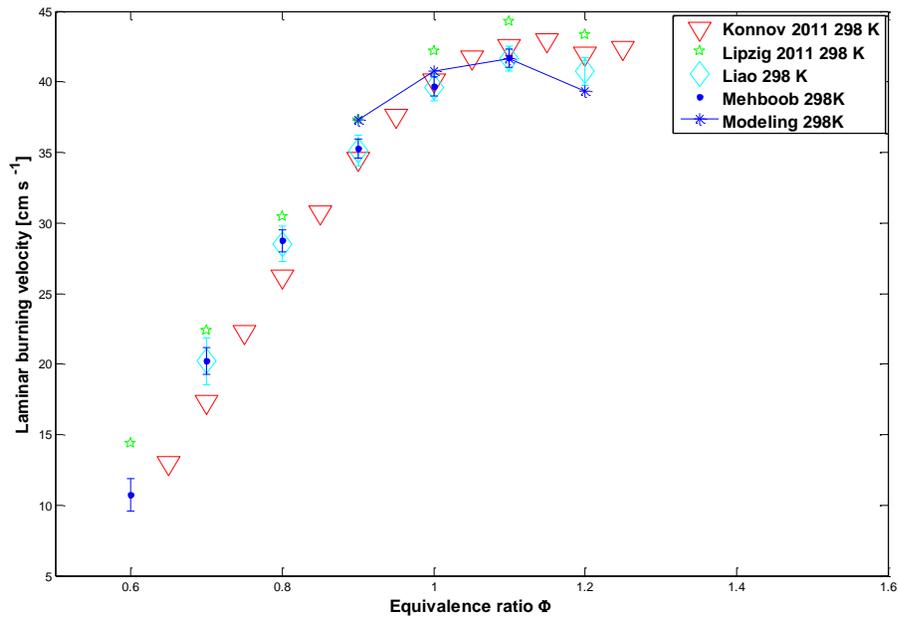


Figure 5.1: Previous experimentally determined flame speeds of ethanol-air flames and the modeling result at 298 K and 1 atm.

As seen in Figure 5.1, Van Lipzing [18] has presented velocities that are higher compared to Konnov [23], Liao [24], Mehboob [25] and the present modeling result. The maximum velocity determined by Konnov is 44.5 cm/s at equivalence ratio, $\Phi = 1.1$. From the graph, it is seen that the current modeling, Mehboob, and Liao present a maximum velocity of 49.5 cm/s is at equivalence ratio 1.1 so their maximum value is overlap almost at the same point and experimental results of Liao et.al are overlapping with Mehboob result. It is known that the measurements of Mehboob have been performed by the heat flux method. There is a good resemblance between the Mehboob results and Liao et al. even if they used different experimental techniques. The entire graph has similar shape and curvature. Good agreements are obtained in its comparison with the modeling velocities with the present and previous literature data.

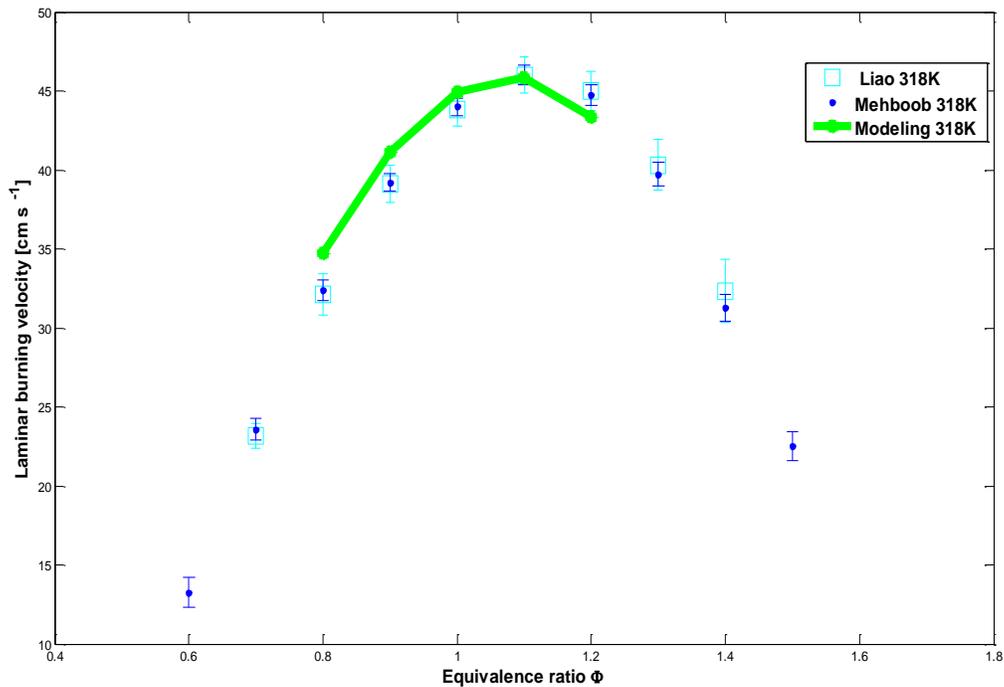


Figure 5.2: Previous and present experimentally determined flame speeds of ethanol-air flames and present modeling result at 318 K at 1 atm.

Figure 5.2, shows that the experimentally determined flame speeds has been compared to the modeled velocities which performed by the CHEMKIN software and the Marinov mechanism. The highest velocity is presented at equivalence ratio 1.1 at 44.5 cm/s. As seen in figure 5.2, almost all experimental values of Liao et.al are overlapping with Mehboob [25] result and their maximum velocity is the same as the peak of the velocity of the modeling result. The highest velocities of the modeling result will be at equivalence ratio 1.1 and the experimental values also peak velocity again at equivalence ratio 1.1. The graph shows the experimentally determined flame speeds compared to those literatures and the modeling result, which tells that at lower equivalence ratios, 0.8-0.9, there is a good correlation between the modeling velocities and the experimental results. Equivalence ratios 0.9-1.0 show a close matching to those of Liao et al. and Mehboob. This suggests that further modeling development is needed to obtain more accurate predictions of the rich side. Generally, the derived modeling results are slightly higher than those presented by Liao et al. and Mehboob except for the 1.2 equivalence ratios.

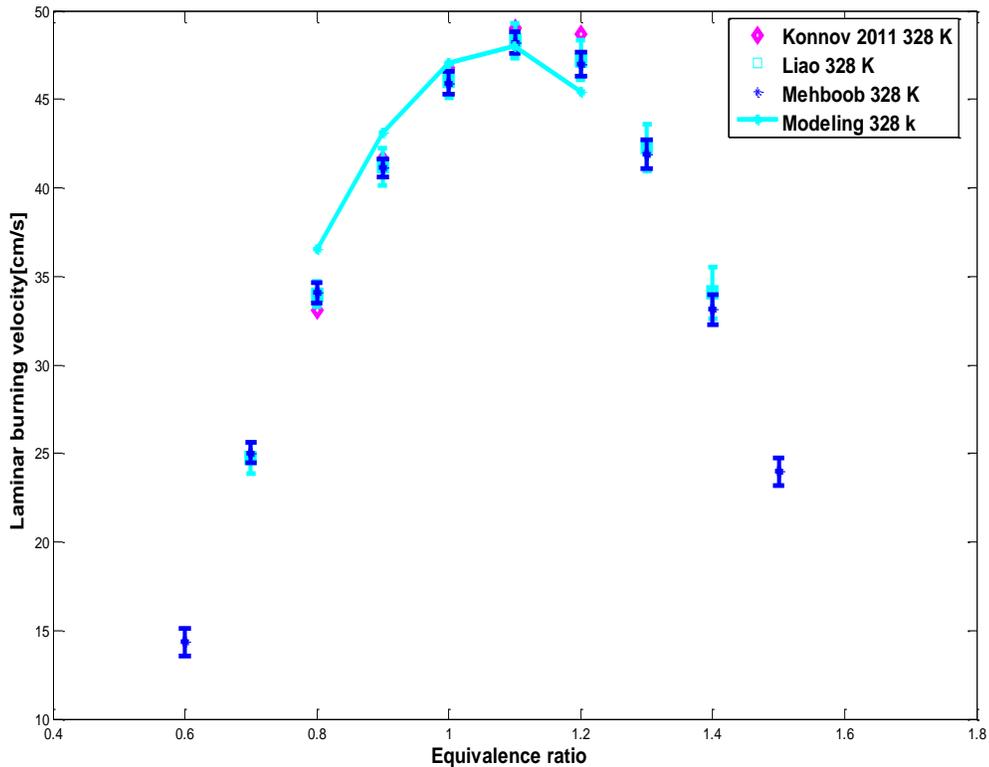


Figure 5.3: Previous and present experimentally determined flame speeds of ethanol-air flames and present modeling result at 328 K at 1 atm.

Figure 5.3 shows the flame speeds at 328 K are measured by Konnov et al, Mehboob, Liao et al, and the present modeling result. There is good agreement between present and previous experimental results in the lean and stoichiometric mixtures. Both groups (Konnov and Liao) and the present modeling result have again presented the highest velocity at 1.1 equivalence ratios. The highest modeling velocity 47.5 cm/s is also presented at 1.1 equivalence ratios and the experimental velocity 45 cm/s also at 1.1 equivalence ratios. The Konnov value 49 cm/s is the highest. Except for the rich mixtures the velocities in the modeling result are higher than all the previous experimental results. The modeled results are slightly higher than the experimental result except at 1.2 equivalence ratios. This shows that there is inconsistency between the modeled and the previously determined flame speeds. This suggests that further modeling development are needed to obtain more accurate predictions of the rich mixture.

Table 5: Summary of peak velocity of ethanol-air

Author	Temperature	Equivalence ratio	Maximum velocity(cm/s)
Konnov et.al	298K	1.15	44.5
	328K	1.1	49
Liao et.al	298K	1.1	38.5
	318K	1.1	44.5
	328K	1.1	47.5
Lipizing et.al	298K	1.1	44.5

5.3 Laminar burning velocity of pure acetaldehyde at different temperature

This section is provided to compare the experimental result and the modeling results of pure acetaldehyde at different temperatures in figures 5.4-5.6. Figure 5.4 shows, the results of the experimental burning velocity of acetaldehyde determined by the heat flux method. The highest experimentally determined burning velocity is at equivalence ratio 1.1 at 50.2, 52.7 and 55.1 cm/s at 338 K, 348 K and 358 K, respectively, but for the temperature 298 K and 318 K the highest burning velocities are 40.9 and 44.5 cm/s respectively at equivalence ratio 1.2. In all experiments the curvatures of the graph at all temperatures are similar to each other; also the maximum burning velocity is reached at equivalence ratio 1.1 for higher temperature but 1.2 for lower temperature. The burning velocities increase with increasing pre-mixture temperature as expected. The error bars indicate that there is a bigger uncertainty for the higher equivalence ratios due to the condensation of the fuel in the evaporator.

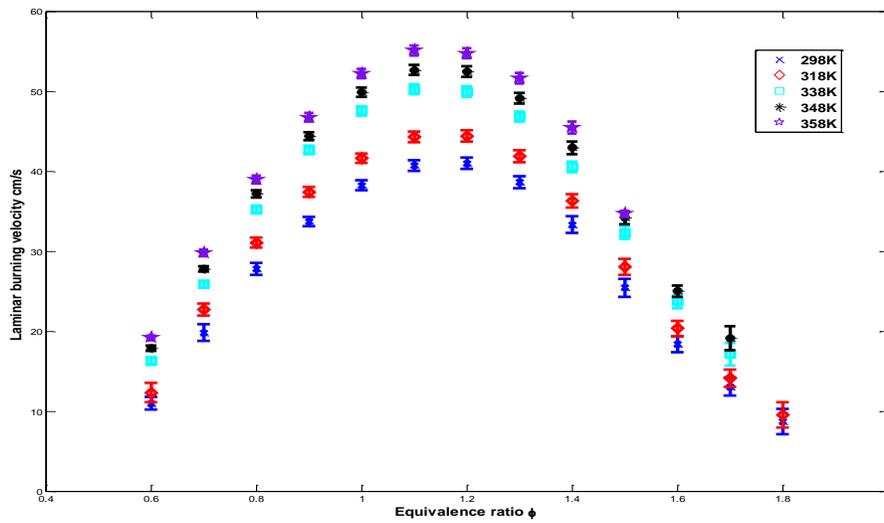


Figure 5.4: Experimental result of acetaldehyde

Figure 5.5 shows the experimentally determined burning velocities compared to those of the literature at 298 K. In the lean mixture, there is good resemblance between the present work and the previous literature of G. J. Gibbs and H. F. Calcote [24] which had been performed by using the Bunsen burner method. The highest velocity of the present work at equivalence ratio 1.2 is 41.5cm/s while the previous literature peak value at equivalence ratio 1.1 is 41.1 cm/se. There is inconsistency between the present work and the previous data in the rich and stoichiometric mixture since they used varying fuel to air ratio and different laboratory conditions. They had also different total flow rate. In the rich mixture the derived velocities of the present work are slightly higher than ones presented by G. J. Gibbs and H. F. Calcote [24].

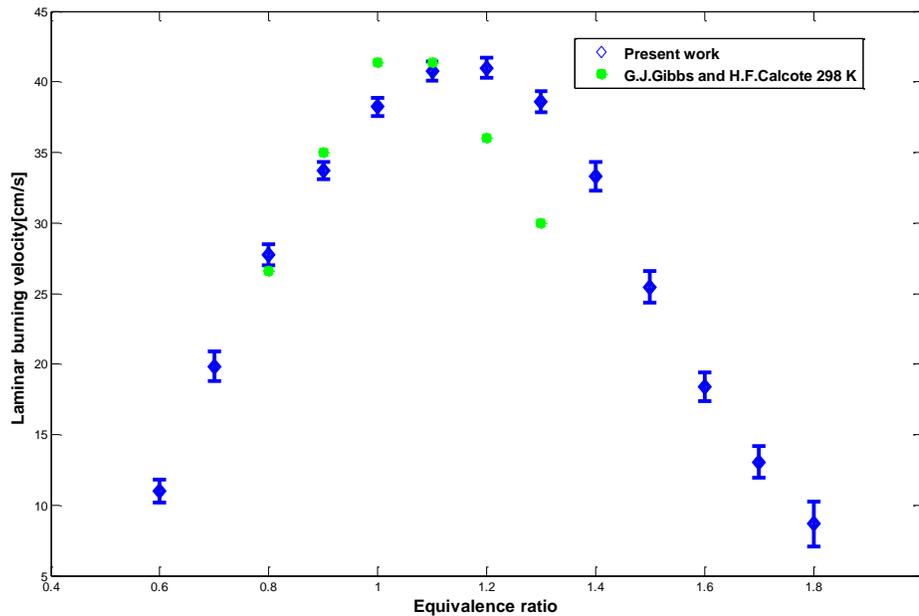


Figure 5.5: Previous experimentally determined flame speeds of acetaldehyde-air flames and present modeling result at 298 K at 1 atm.

Figure 5.6 shows the experimentally determined burning compared to that of the modeling results. The highest flame speed of the modeled result is at equivalence ratio 1.1, is 45.6, 47.85, 53.6 and 59.3 cm/s for the corresponding temperature, 298 K, 318 K, 338 K and 358 K respectively. The results can be compared to the experimentally determined burning velocity is at equivalence ratio 1.1 at 50.2, 52.7 and 55.1 cm/s at 338 K, and 358 K respectively but for the temperature 298 K and 318 K the highest burning velocity is 40.9 and 44.5 cm/s respectively at equivalence ratio 1.2. As seen in the figure the calculated (modeling) burning velocity of the acetaldehyde is higher than the measured (experimental) values, for the corresponding temperature. However, the position of the peak and the shape of the curvature are well reproduced. The modeled velocities all have the highest velocity at equivalence ratio 1.1 while the experimental values all peak at equivalence ratio 1.1 for higher temperature but 1.2 for the lower temperature. Almost all the shape of the curvatures of the modeling result at all temperatures is similar to each other, as well the experimental result having similar shape and curvature.

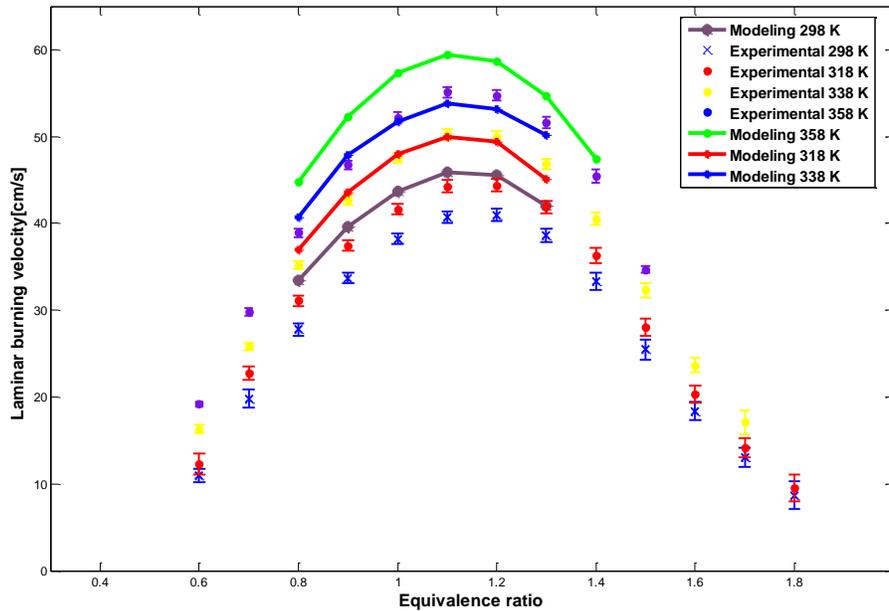


Figure 5.6: Measured adiabatic burning velocities and modeling results of acetaldehyde at different temperature.

The burning velocities increase with increasing pre-mixture temperature as expected. Figure 5.6 shows that there is inconsistency between the modeled and the measured values. This suggests that further modeling development is needed to obtain more accurate predictions of the lean and rich mixture. There is only one reference about laminar burning velocity of acetaldehyde is presented by G. J. Gibbs and H. F. Calcote. In order to validate the experimental results, a comparison has to be made only with the modeling results that have been carried out here.

5.4 Laminar burning velocity of the ethanol-acetaldehyde mixtures at different temperature

As seen in figure 5.7, the burning velocity of the ethanol-acetaldehyde mixture at 298 K unburnt gas temperatures. In the figure the experimental values of the pure ethanol is overlapping its results with 20% acetaldehyde mixture. At lower equivalence ratios the modeled results are higher than the experimental result. The maximum flame speed of the modeling result is observed at equivalence ratio 1.1. The highest experimental result also determined the flame speed of 20% acetaldehyde mixture is 35.5 cm/s at equivalence ratio 1.0. Also, the maximum burning velocity both in the present modeling result of 20% acetaldehyde mixture and the present experimental result of a pure ethanol is 42.7cm/s at equivalence ratio 1.1. This suggests that further modeling and experiment development are needed to obtain more accurate predictions of the rich mixture.

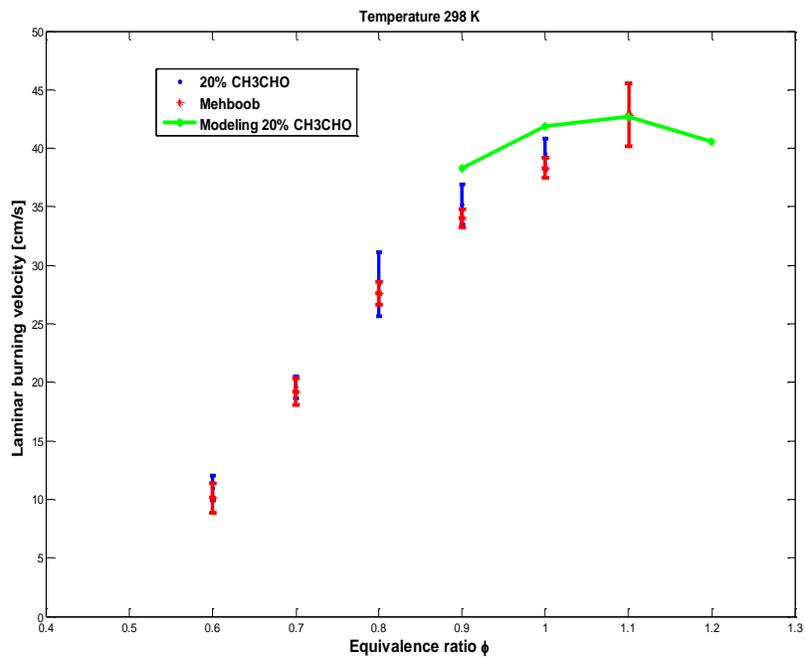


Figure 5.7: Experimental results of 20 % acetaldehyde, the measured burning velocities of ethanol and the modeling result 20 % acetaldehyde.

Figure 5.8 shows the experimentally determined flame speeds compared to those of Mehboob results at 298 K. At all equivalence ratios, there is a good correlation between the present velocities 10% acetaldehyde and Mehboob result. Equivalence ratios 0.9-1.1 the modeling result is a close match to the experimental result. The derived modeled results are slightly higher from the experimental result.

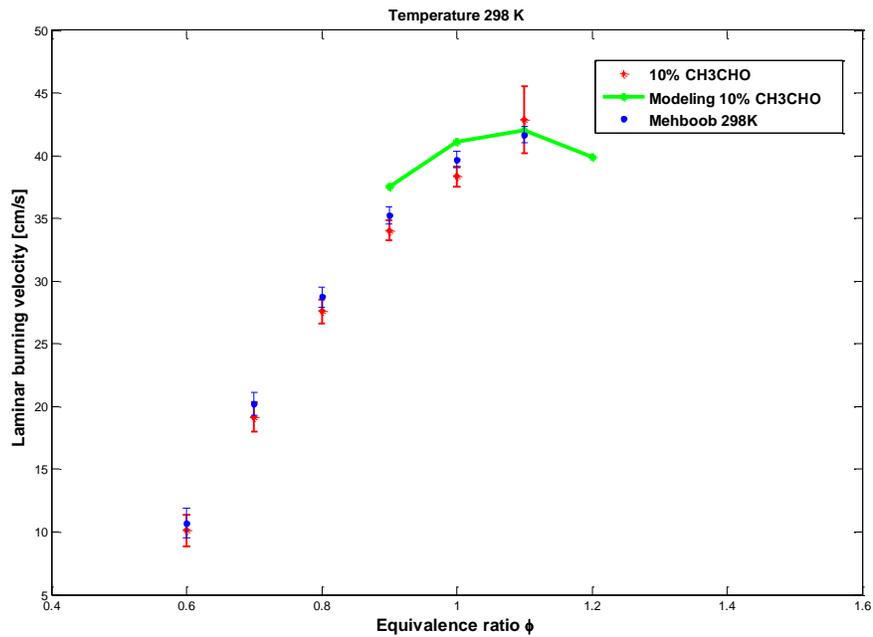


Figure 5.8: Experimental results of 10 % acetaldehyde, the measured burning velocities of ethanol and the modeling result 10 % acetaldehyde.

Figure 5.9 shows the 50 % of acetaldehyde experimentally determined burning velocities compared to those of modeling results. The highest flame speed of the modeled result at 1.1 equivalence ratios is 43.8 cm/s and 48.08 cm/s, for the corresponding temperature, 298 K, and 318 K, respectively. The results can be compared to the experimental velocity at the 1.1 equivalence ratio is 41.5 cm/s and 43.75 cm/s, at 298 K, and 318 K, respectively. As seen in figure 5.9, the calculated (modeling) burning velocities of the 50 % acetaldehyde are higher than the measured (experimental) values for the corresponding temperature. The modeled and experimental reaches their peak value at equivalence ratio 1.1. At lower equivalence ratio, the experimental result in both temperatures becomes overlap.

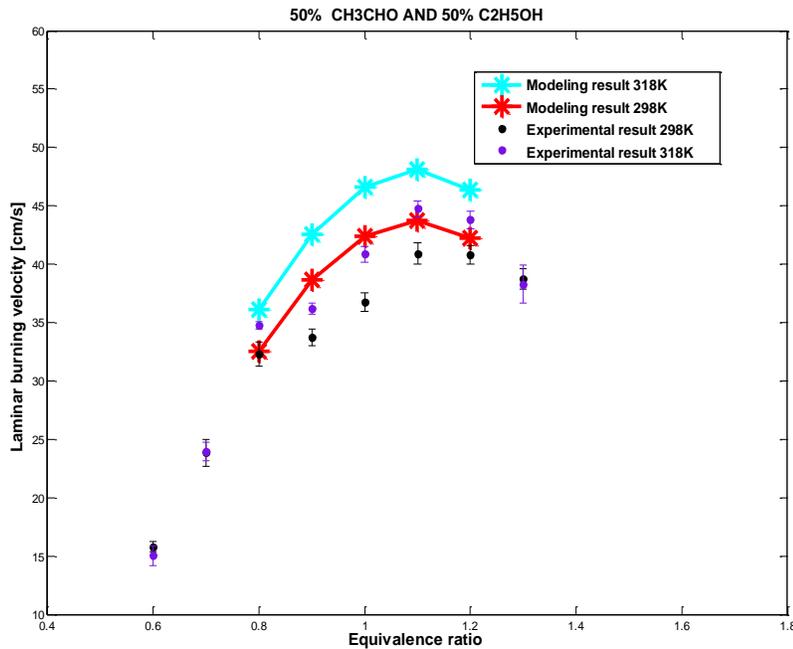


Figure 5.9: The modeling and the experimental result of 50% of acetaldehyde with ethanol

Here is also, no literature data exist regarding the laminar burning velocity of the study of the 50 % acetaldehyde mixture. In order to validate the experimental results, comparison has to be made only with the modeling results that have been carried out.

5.5 Temperature correlations with laminar burning velocity.

In this section is discussed the characteristics of the burning velocity on the unburnt gas mixture temperature of acetaldehyde at various equivalence ratios in a temperature range of 298 -358 K .The water baths are used in the present setup to keep the temperature of the burner plate and plenum chamber. These two water baths were set to at temperatures between in the range of 25-85 °C. A burner plate is fixed at a temperature of 368 K. As the principle of the heat flux method the temperature of unburnt gas mixture in plenum chamber is kept constant and it will be discussed in the following section to obtain reasonable stable flame. Furthermore, for the application of the heat flux method as described in this work, it is necessary that the water jacket keeps the edge of the burner plate. It is known that the adiabatic laminar burning velocity, S_L is characteristic of a fuel mixture and dependent on various properties; temperature, pressure, and equivalence ratio. The most widely used correlation describing the effect of unburnt gas temperature on the flame speed is given in equation 5.1:

$$S_L = S_{L,0} \left(\frac{T_u}{T_0} \right)^{\alpha_T} . \quad \dots\dots\dots 5.1$$

where, T denotes temperature of the mixture. The subscript u denotes the unburnt gas conditions. The parameter α_T depends on equivalence ratio; which can be determined by finding the slope.

Similarly, Equation 5.1 can also be used for numerical calculations if it is written in other form. By using a simplified form of the power law stated given in relation 5.2.

$$S_L \sim T_u^{\alpha_T} \quad \text{..... 5.2}$$

The linear relation between burning velocity and temperature on a log-log scale is obtained as result the power exponent α is a factor derived from the temperature dependence of the laminar burning velocity. It is determined by measuring the slope of each line at various equivalence ratios. The temperature correlation with burning velocity for all acetaldehyde is used in this project will be presented in this section as well as power exponent coefficients against equivalence ratio for acetaldehyde will be also described here.

Figure 5.10 on log-log scale shows the relation between of the adiabatic burning velocity of acetaldehyde-air flames and unburnt gas temperatures for several equivalence ratios at ambient pressure. The symbols represent experimental data. It is evident that the coefficient (α_T) corresponds to the slope of the line in the figure at each equivalence ratio. Figure 5.11 shows the coefficients α_T (in equation (5.1)), determined by the slopes of the lines in Figure 5.10, versus equivalence ratio.

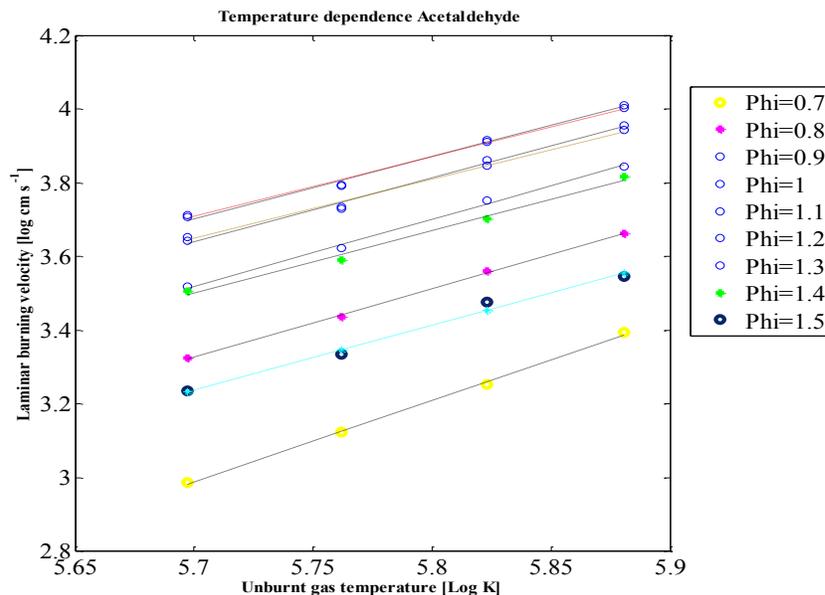


Figure 5.10: Temperature dependence of acetaldehyde burning velocity in the range 298 - 358 K, plotted on a log- log scale.

Figure 5.10 shows linearly fitted graphs. According to the above figure, it is possible to say that the coefficient shows linear behavior. The unburnt gas temperature has a good match to the linear fit. From the slope of the linear fit seen in figure 5.10 the power exponent α is derived. As seen in figure 5.11 a minimum coefficient value is observed at an equivalence ratio at 1.2 and 1.3. The error bars are derived by adding the deviation in burning velocity at temperature ranges (298 -358 K). From the maximum and minimum slope from the single graphs can be determined which correspond to the deviation in coefficient α_T . Obviously this has to be done for each equivalence ratio. These coefficients can be plotted in terms their corresponding equivalence ratios (0.8-1.5), as seen in Figure 5.11. The error bars of the present work are derived due to the error of the individual flame speed measurements at different temperatures. The errors in power exponent determined for each equivalence ratio based on the errors from the laminar burning velocity curve to calculate these errors from the figure 5.11 it has to be considered the following procedure .

First calculate the slope (α_0) for the line, then take two extreme points i.e. the maximum and minimum slope from the single error bar can be determined which correspond to the deviation in coefficient α_0 on the error bar then determine their slope which are α_1 and α_2 . At last determine the standard deviation α_0 α_1 and α_2 .

The error bars are obtained by taking the mean and standard deviation of errors for different coefficients, by using the following relations.

$$\bar{\alpha} = \frac{1}{n} \sum_{i=0}^n \alpha_i \quad \dots\dots\dots 5.3$$

$$s = \left(\frac{1}{n-1} \sum_{i=0}^n (\alpha_i - \bar{\alpha})^2 \right)^{\frac{1}{2}} \quad \dots\dots\dots 5.4$$

Where n is the number of coefficients and index i stands for different measured points. The figure 5.11 with error bars are shown and discussed for each equivalence ratio.

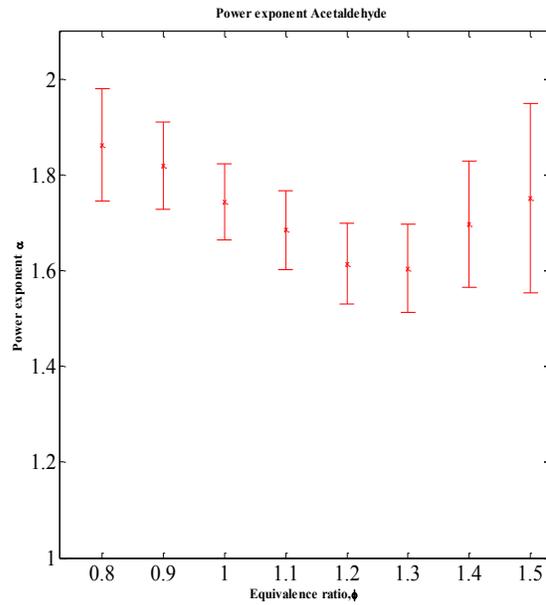


Figure 5.11: Power exponent versus equivalence ratio Acetaldehyde.

To compare the present result of coefficient against equivalence ratio, no literature data exist regarding to acetaldehyde. As displayed figure 5.11, it shows that the experimental error bar becomes larger at equivalence ratio of 1.5. The scattering of experimental values of α , is too large to draw any certain conclusions of its relationship to Φ . The uncertainty of the power exponent is very high for the small temperature range; in order to increase the accuracy of coefficients, the temperature range must be increased.

Chapter 6 Conclusion and Recommendation

The heat flux method has been performed to measure the adiabatic burning velocity of liquid fuel. The primary goal of this study is to provide new and accurate measurements of the laminar burning velocities of acetaldehyde, ethanol and ethanol-acetaldehyde mixture by using this method. The measurements have been carried out at various temperature range of (298 K -358 k) and equivalence ratio range of (0.6-1.8). These results have been validated with modeling by using the Marinov Mechanism (1999) and previous work. The modeled derived burning velocities of ethanol using the Marinov Mechanism (1999), has been validated by using the previous work. There is inconsistency between the modeled and the previously determined flame speeds of pure ethanol but there is a good correlation between the present experiment and the previous work. The burning velocities determined for acetaldehyde by this method have been validated by using the modeled results, figure 5.1-5.6. The burning velocities of acetaldehyde/air flames were compared with respect to each other and their modeling result since there is no literature data available to compare with. The Marinov Mechanism has been implemented in the CHEMKIN package. Calculated burning velocities show somewhat higher values although a good qualitative shape of the curve was reproduced. Likewise to acetaldehyde, burning velocities were measured at elevated temperatures over a similar range of (298 K - 358 K). The modeled velocities all have the highest velocity at equivalence ratio 1.1 while the experimental values all peak at equivalence ratio 1.1 for higher temperature but 1.2 for the lower temperature. As seen the calculated (modeling) burning velocities of the acetaldehyde are higher than the measured (experimental) values, for the corresponding temperature. This suggests that further modeling development is needed to obtain more accurate predictions of the rich mixture. Temperature and burning velocity have been correlated by a power law over several ranges of equivalence ratios. There is an increasing flame speed with increasing of temperature. It is a fairly good agreement between the experimental results and the derived modeled velocities. The burning velocities of the different percentage of ethanol-acetaldehyde mixtures are presented in Figures 5.7-5.9. The experimentally determined burning velocities have a good agreement with the modeled result for lower equivalence ratios. The experimental values of the pure ethanol are overlapping its results with 10% and 20 % acetaldehyde mixture. Figure 5.9 indicates that there is a discrepancy in the shape of the curvature of the graph of experimental and modeling results at 298 K and 318 K for 50% acetaldehyde. However, the maximum velocity of the model and experiment results is determined at the same equivalence ratio $\Phi = 1.1$ as shown in figure 5.9. No literature data exist regarding the laminar burning velocity of the study of the 50 % acetaldehyde mixture. This suggests that further experiment and model development are required especially at the rich mixture.

Some recommendations can be considered to improve the experimental setup:

- More experiment can be performed by using another method, for example, Bunsen burner method or Counter flow methods for comparing the results with heat flux method.
- More experiment and modeling with different mixtures have to be carried out to examine the reliability and the validity of the results.
- A heating tube could be used to keep the temperature of the unburned mixture. Therefore, combustion of ethanol, acetaldehyde and their mixture can be measured.
- A new kinetic modeling mechanism could be designed for acetaldehyde, ethanol and ethanol-acetaldehyde mixture other than Marinov mechanism.

A higher level of accuracy can be reached if the above mentioned recommendations are applied.

Reference

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Appendix A Tabulated adiabatic burning velocities

This appendix is contained the measured value of adiabatic burning velocities of acetaldehyde using the heat flux method are listed in tables. The experimental data is presented together with corresponding error estimates. The measurements are performed at ambient pressure which is 1 atm. The unburnt gas mixture temperature is varied over a range of 298 K – 358 K

1 Acetaldehyde

T= 298 K

Equivalence Ratio(Φ)	Laminar flame speed(S_L)	Uncertainty(Φ)	Uncertainty(S_L)
0.6	10.99	0.0128	0.7980
0.7	19.83	0.0150	1.0510
0.8	27.77	0.0171	0.7569
0.9	33.70	0.0192	0.59051
1.0	38.23	0.0214	0.6363
1.1	40.73	0.0235	0.6679
1.2	40.97	0.0256	0.7102
1.3	38.60	0.0278	0.7399
1.4	33.32	0.0293	1.0142
1.5	25.45	0.0320	1.1249
1.6	18.38	0.0342	1.0067
1.7	13.04	0.0363	1.1249
1.8	8.67	0.0385	1.5821

T=318 K

Equivalence Ratio(Φ)	Laminar flame speed(S_L)	Uncertainty(Φ)	Uncertainty(S_L)
0.6	12.31	0.0122	1.2036
0.7	22.73	0.0142	0.7526
0.8	31.07	0.0162	0.6106
0.9	37.41	0.0183	0.5990
1.0	41.64	0.0203	0.5985
1.1	44.29	0.0223	0.6712

1.2	44.39	0.0243	0.7086
1.3	41.87	0.0264	0.7617
1.4	36.28	0.0284	0.8503
1.5	28.06	0.0304	0.9813
1.6	20.35	0.0325	0.9745
1.7	14.14	0.0345	1.1049
1.8	9.53	0.0365	1.5631

T=338 K

Equivalence Ratio(Φ)	Laminar flame speed(S_L)	Uncertainty(Φ)	Uncertainty(S_L)
0.6	16.30	0.0094	4.8985
0.7	25.89	0.0110	3.7140
0.8	35.20	0.0126	3.4809
0.9	42.65	0.0141	3.5119
1.0	47.53	0.0157	3.2585
1.1	50.24	0.0173	3.6224
1.2	49.99	0.0188	3.6926
1.3	46.83	0.0204	3.7473
1.4	40.54	0.0220	4.4910
1.5	32.33	0.0236	5.7761
1.6	23.68	0.0251	6.5504
1.7	17.09	0.0267	11.6826

T=348 k

Equivalence Ratio(Φ)	Lamina flame speed(S_L)	Uncertainty(Φ)	Uncertainty(S_L)
0.6	17.90	0.0091	0.4216
0.7	25.88	0.0110	3.7140
0.8	37.18	0.0121	0.5260
0.9	44.40	0.0136	0.5636
1.0	49.90	0.0152	0.6299
1.1	52.67	0.0167	0.7080
1.2	52.45	0.0182	0.7213
1.3	49.12	0.0197	0.6906
1.4	42.93	0.0212	0.8412
1.5	34.19	0.0227	0.8496
1.6	25.00	0.0242	0.7207
1.7	19.12	0.0258	1.5576

T = 358 K

Equivalence Ratio(Φ)	Laminar flame speed(S_L)	Uncertainty(Φ)	Uncertainty(S_L)
0.6	19.18	0.0079	0.4979
0.7	29.80	0.0092	0.6001
0.8	35.20	0.0126	3.4809
0.9	46.75	0.0119	0.6548
1.0	52.21	0.0132	0.6997
1.1	55.09	0.0145	0.7454
1.2	54.75	0.0158	0.7548
1.3	51.60	0.0172	0.7730
1.4	45.42	0.0185	0.8552
1.5	34.68	0.0198	0.5702

Appendix B : Mat lab script to calculate the numerical data of modeling results.

```
%% This file plots flame speed vs equivalent ratio .....

equivalentratio=.8:.1:1.4;

eq08=importdata('eq0.8.csv');
speed08=eq08.data(:,4);
eq09=importdata('eq0.9.csv');
speed09=eq09.data(:,4);
eq10=importdata('eq1.0.csv');
speed10=eq10.data(:,4);
eq11=importdata('eq1.1.csv');
speed11=eq11.data(:,4);
eq12=importdata('eq1.2.csv');
speed12=eq12.data(:,4);
eq13=importdata('eq1.3.csv');
speed13=eq13.data(:,4);
eq14=importdata('eq1.4.csv');
speed14=eq14.data(:,4);
eq15=importdata('eq1.5.csv');
speed15=eq14.data(:,5);

speed=[speed08(1,:) speed09(1,:) speed10(1,:) speed11(1,:) speed12(1,:)
speed13(1,:) speed14(1,:) speed15=eq14.data(:,5)];
plot(equivalentratio, speed, '*g')
xlabel('equivalent ratio')
ylabel('flame speed')
title('flame speed vs equivalent ratio').
clear all
clc
```

C : Mat lab script is used to calculate figure 3.7

```
lear all
clc
A=importdata('eq0.9.txt','\t',22); %import the data without text
r=A.data(:,2); %radial
T=A.data(:,3); %Temp.
n=7; % The number of data values for each alpha value
lincolr='rrrrrrrrggggggggbbbbbbkkkkkkkk'; % colors of the lines in the
figures
figure(1)
for i=1:8:32
%TT=[T(i) T(i+n-6) T(i+n-5) T(i+n-4) T(i+n-3) T(i+n-1) T(i+n-0)];% (T(i+n-
3)+T(i+n-1))/2 ;%T(i:i+n);
%rr=[r(i) r(i+n-6) r(i+n-5) r(i+n-4) r(i+n-3) r(i+n-1) r(i+n-0)];% (r(i+n-
3)+r(i+n-1))/2 ;
%TT=T(i:1:i+n);
%rr=r(i:1:i+n);
%TT=[T(i) T(i+n-6) T(i+n-5) T(i+n-4) T(i+n-3) T(i+n-2) T(i+n-1) T(i+n-
0)];%T(i:i+n);
%rr=[r(i) r(i+n-6) r(i+n-5) r(i+n-4) r(i+n-3) r(i+n-2) r(i+n-1) r(i+n-0)];
% all
TT=[T(i) T(i+n-6) T(i+n-5) T(i+n-4) T(i+n-3) T(i+n-1) T(i+n-0)];%T(i:i+n);
rr=[r(i) r(i+n-6) r(i+n-5) r(i+n-4) r(i+n-3) r(i+n-1) r(i+n-0)]; % without
THERMOCOUPLE SIX
fit=regstats(TT,rr.^2);
fitbeta=fit.beta;
T0=fitbeta(1);
alpha=fitbeta(2);
tdist=T0+alpha*rr.^2;
h=plot(rr,TT,'*- ',rr,tdist,'LineWidth',2);
set(h,'Color',lincolr(i), 'LineWidth',1);
xlabel ('radial');
ylabel('Temperature ');
hold on
end
grid on

legend('\alpha^2=-0.016112','\alpha^2=-0.016112','\alpha^2=-0.005351',...
'\alpha^2=-0.005351','\alpha^2=0.004129','\alpha^2=0.004129',...
'\alpha^2=0.015928','\alpha^2=0.015928')
```