Final Report

Autoignition and Combustion of Biofuels

Research project at the University of California at San Diego

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Chapter 1

Introduction

Gasoline and Diesel are the main source of energy for transportation in most developed countries. These are fossil fuels derived from crude oil which is a finite resource. Since the price for crude oil steadily increased in the near past and is likely to rise in the future, the dependancy on and the security of supply has become an important topic.

Governments want to lower the dependancy on crude oil and so several alternatives are explored. An easier way of changing the fuel source than introducing new fuels onto the market is to blend fuels derived of renewable sources into common liquid fuels. Therefore the United States legislator introduced laws, demanding renewable fuels to be mixed into petroleum-derived fuels. Among others this includes ethanol made from biomass.

Increasing concentrations of ethanol blended into regular gasoline calls for an investigation on how this affects the combustion behavior. Gasoline itself is made up of hundreds of hydrocarbons and a great variety of chemical reactions take place during combustion. A detailed model for numerical calculations of combustion would be too large and would lead to long computing times. Therefore surrogates, reproducing certain selected characteristics of combustion of gasoline are used to build semi-detailed chemical-kinetic mechanisms. Reliable experimental data is

needed in order to test and calibrate the used kinetic models of combustion.

In the work reported here critical conditions of extinction and autoignition are measured for blends of a developed surrogate for gasoline and ethanol. These experimental results were compared to those of similar blends of gasoline and ethanol to prove the reproduction of combustion characteristics.

1.1 Ethanol

Ethanol, also called ethyl alcohol, has the molecular formula C_2H_5OH. Due to the oxygen molecule it is a partially oxygenated hydrocarbon and has a lower energy density by mass ($\sim$30 MJ/kg) compared to the similar but non-oxidized ethane (C_2H_6; 47 MJ/kg) or Gasoline ($\sim$44 MJ/kg) [1].

The hydroxyl group at the end of a straight chain alcohol molecule has a big influence on its physical properties and behavior in chemical processes. Due to the polarity, ethanol is less volatile than short chain hydrocarbons like ethane through pentane. Unlike gasoline it is miscible with water. Mixing ethanol into a gasoline makes it hydroscopic to a moderate extent.

Ethanol has a research octane number of 110 and thus raises the octane number of gasoline when being mixed into. It oxygenates the fuel and thereby lowers the forming of Volatile Organic Compounds (VOC) and carbon monoxide while combustion in engines. Since it is blended into gasoline in the United States it is about to replace the octane enhancer methyl tertiary butyl ether (MTBE) completely.

1.2 Gasoline

Gasoline is derived from crude oil and therefore does not have a uniform composition. It is a mixture of hundreds of hydrocarbons each with its specific properties.

Due to its mixture of volatile and more viscous components, it has a wide boiling curve reaching from about 25°C to 210°C. During the combustion process of gasoline thousands of chemical reactions take place.

To describe the combustion of gasoline, the chemical-kinetic mechanisms of its components have to be found. Numerical calculations on combustion of gasoline are very complex as many chemical-kinetic mechanisms exist. The simple assembling of the mechanisms of its components leads to a too large mechanism for gasoline and cannot be computed.

The uncertain content of ethanol in regular gasoline and its variing composition depending on its source call for a well defined fuel guaranteeing repeatability of experiments. The fuel used for the experiments in this study is the unleaded test gasoline UTG-96, provided by Chevron Phillips Chemical Company LP. It is a emission certification fuel, meeting the requirements outlined in Code of Federal Regulation 40 CFR, Part 86.1313, for use in CAFE and Emission Certification Testing. Its content of ethanol and other oxygenates ist 0.0% and it is unleaded. Its properties are summarized in Table 1.1 [2].

Table 1.1: Properties of the Emission Certification Gasoline UTG-96.

Research Octane Number	Motor Octane Number	Anti-Knock Index RON+MON/2	Density (kg/m^3) at 298 K	Energy Density (MJ/kg)
96.5	87.7	92.1	740.9	42.56

To compare and assure the results derived with UTG-96 certain data points of the experiments were also done with common gasoline from a local gas station. From here on the gas station gasoline will be refered to as "Gasoline91" and the emission certification fuel as "UTG96".

1.3   Surrogate

Due to the variety of different chemical reactions in the burning process of gasoline, numerical calculations of combustion is difficult. Developing surrogates made up of only some hydrocarbons can be an approach. These surrogates are designed to reproduce selected characteristics of combustion of the gasoline. The chemical-kinetic mechanism for the used components are well known and the computational time keeps within reasonable limits. [3]

By comparing results of experiments on a certain gasoline and its surrogate, similar characteristics can be proved. Detailed mechanisms for combustion of the surrogates are much simpler and can be used in computations. Numerical calculations on combustion of the surrogate can be done and veryfied with the experiments.

Surrogates made out of *n*-heptane and *iso*-octane are used to define the knock behaviour of combustion of gasoline in internal combustion engines. These mixtures are called primary reference fuels (PRF) and are used for the octane rating of gasoline. Pure *n*-heptane represents an octane number of 0, *iso*-octane has an octane number of 100. In a specific test a gasoline of a octane number of X behaves the same way a mixture of X% iso-octane and (100-X)% n-heptane does. The most common octane rating is the research octane number (RON), being determined with a test engine at low speed and low load. For the motor octane nuber (MON) higher speeds and more load are used. Although the testing procedures are similar, these two ratings already can be very different for one gasoline as already seen in Table 1.1. As knocking is a matter of autoignition, this shows that a surrogate with only these two components does not reproduce the autoignition behaviour of a gasoline adequate.

n-heptane and *iso*-octane represent the behaviour of straigth chain and branched alkanes, respectively. To account for aromatics and cycloalkanes in gasoline further components in the surrogates have to be used. The surrogate of gasoline used in the experiments described in this study is taken from this previous study [3]. See

Table 1.2 for the composition and properties of the employed components. This

Table 1.2: Surrogate composition and properties of employed components.

	vol% at 298 K	Mole%	Chemical Symbol	Molecular Weight (g/mol)	Density (kg/m³) at 298 K
n-Heptane	20	19.29	C_7H_{16}	100.21	683
iso-Octane	40	34.10	C_8H_{18}	114.23	688
Toluene	10	13.32	C_7H_8	92.14	867
Methylcyclohexane	30	33.30	C_7H_{14}	98.19	770

four-component surrogate was found to best reproduce the combustion characteristics of gasoline. It is composed of the straight-chain alkane *n*-heptane, *iso*-octane (also referred to as 2,2,4-Trimethylpentane), the aromatic compound toluene and the cycloalkane methylcyclohexane.

1.4 Counterflow Configuration

The experimental setup is different to an internal combustion gasoline engine. In engines gasoline is burned discontinuous in a cylinder in turbulent ambient with varying pressure and temperature. Gasoline is injected into the inflowing air or directly into the cylinder where vaporization takes place. While still being compressed, a spark plug ignites the fuel-air mixture and the flame proceeds through the highly turbulent environment.

The experiments are carried out using the counterflow setup as seen in Figure 1.1 [4]. Two ducts, called oxidizer-duct and fuel-duct, sit opposite to one another. On each side a laminar flow leaves the duct and stagnates against the flow of the opposed duct, leading to a special flow field. Pure air or air dilluted with nitrogen enters through the upper oxidizer-duct, called oxidizer boundary, and vaporized fuel together with nitrogen enter through the lower fuel-duct, also called fuel boundary. The combustion zone is guided by a nitrogen-curtain and the combustion gases are sucked off. The fuel is vaporized in an external vaporizer, so
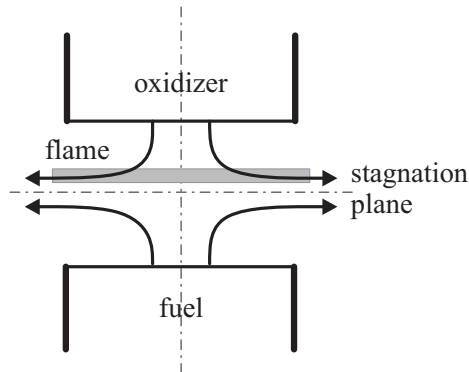
Figure 1.1: Schematic illustration of a nonpremixed laminar counterflow configuration.

all participants are gases.

By diffusion the oxidant and the fuel form a flammabe mixture in a narrow region around the stagnation plane. Thus an established flame is called a non premixed diffusion flame. A diffusion flame establishes always at the place of maximum energy output, thus at the place with stoichiometric conditions [4].

1.4.1 Strain Rate

The strain rate is used to characterize the flow field in the counterflow setup. It is defined as the normal gradient of the normal component of the flow velocity. It is obtained from an asymptotic theory where the Reynolds numbers of the laminar flow at the boundaries are presumed to be large [5]. It changes from one duct exit to the other. The strain rate a_2 on the side of the oxidizer duct of the stagnation plane is given by equation 1.1.

$$a_2 = \frac{2\,|V_2|}{L}\left(1 + \frac{|V_1|\,\sqrt{\rho_1}}{|V_2|\,\sqrt{\rho_2}}\right)$$ (1.1)

The subscript 1 denotes for conditions at the fuel side, whereas 2 stands for conditions at the oxidizer side of the stagnation plane. L is the distance between the two opposing ducts, V_1, V_2 and ρ_1, ρ_2, are the components normal to the stagnation plane of the velocities and the densities, all at the according duct exits.

1.5   Ignition and Extinction

The points of autoignition and extinction of a diffusion flame in the counterflow setup are the two burning limits which are investigated in the experiments.

When there is no flame, the flow is considered frozen without appreciable chemical reactions. Autoignition can be reached either by decreasing the strain rate or increasing the maximum temperature of the stream. At a certain point the chemical ractions take place leading to autoignition. The temperature immediately rises and a flame is established. In the experiments autoignition is achieved by increasing the maximum temperature at a constant strain rate.

An established flame can be extinguished by increasing the strain rate. As the strain rate incrases, the time for chemical reactions becomes shorter. At the point of extinction the maximum temperature instantaneous decreases.

Chapter 2

Experimental Setup

The experimental setup as seen in Figure 2.1 consists of the burner itself, a vapor-
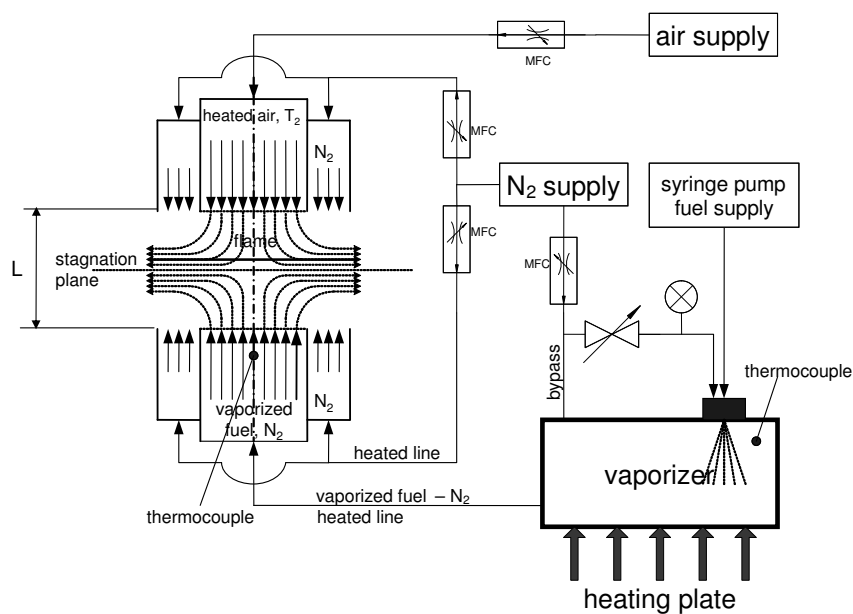

Figure 2.1: Schematic illustration of the experimental setup. The figure shows the counterflow flow field and the air, nitrogen, and fuel feed systems and the vaporizer.

izer, the gas and fuel supply and the measuring and controlling equipment. The

burner is built from an upper and a lower part which can be exchanged modu-

larly for different types of experiments. All parts are axissymetric and aligned

centrically to obtain a axially symmetric flow.

2.1 Lower Part of Burner

In the performed nonpremixed, prevaporized experiments the lower part of the burner has a center fuel-duct with diameter of 23.1 mm. It is surrounded by the annular curtain duct, providing a nitrogen curtain to screen the reaction zone from the environment. The combustion gases are sucked into the outlying exhaust, where six spray nozzles inject water to prevent further reaction.

2.2 Upper Part of Burner

For autoignition and extinction there are two exchangeable burner tops, accounting for the different needs. Each top is connected to the lower part of the burner via three adjustable pins for setting the duct distance and fast exchange.

2.2.1 Oxidizer for Autoignition Experiments

The autoignition top has a centric oxidizer duct, diameter 22.3 mm, made of quartz for little heat expansion. It is surrounded by a quartz curtain duct and an insolation. A silica carbide resistance coil heats the oxidizer stream and can be controlled by a autotransformer. It can be aligned precisely in the axis to assure an axyssymetrical heating. The metal parts at the outer duct are cooled with water. For autoignition the distance between fuel and oxidizer duct is $L = 12$ mm.

2.2.2 Oxidizer for Extinction Experiments

The extinction top consists of a centric oxidizer duct, diameter 23.0 mm, and a surrounding curtain duct, both made of steel. No heating and cooling is necessary.

The distance between fuel and oxidizer duct for the extinction experiments is $L=$ 10 mm.

2.3   Vaporizer

The vaporizer is situated upstream from the fuel-duct and provides a steady flow of vaporated fuel well mixed with nitrogen. The bottom is heated by a heating plate, the walls are insolated and heated with a heating tape, controlled by a autotransformer. A nozzle injects liquid fuel together with gaseous nitrogen, supporting the fragmentation of the fuel stream.

The flow line from the vaporizer to the fuel duct and the lower curtain supply are heated to prevent condensation and to asure equal temperatures in duct and curtain.

2.4   Gas and Fuel Supply

Nitrogen is stored in several gas zylinders with 150 bar initial pressure and compressed air is provided in-house. Pressure reducing valves provide a steady supply pressure. On a panel flowmeters and pressure gauges show the state of the flows.

The feed of the system with fuel is done by a syringe pump. Two syringes filled with fuel are mounted in the syringe pump and the volume flow is set by selecting a gear.

2.5   Controlling Software

All gas flowes are controlled by a computer. A programm written in C++ calculates out of the setup properties and the desired values the flow controller settings.

The program takes the dimensions of all ducts, the properties of all gases and fuels and the temperatures at the exits of the ducts into account.

2.6   Mass Flow Controllers

The controlling software calculates the proper settings for the mass flow controllers, witch are cable connected to the computer. The used MFCs provide a mass flow linear to the impressed voltage. The integrated sensor in the MFC provides the information for closed loop control of the integrated control valve.

2.7   Temperature Measurement

Thermocouples measure the temperature at several measuring points. In autoignition experiments a type R (platinum-13%rhodium vs. platinum) thermocouple is used between the two ducts directly next to the oxidizer-duct. The measured oxidizer temperature is corrected for radiation loss.

2.8   Exhaust System

A slight vaccuum sucks the combustion gases through the exhaust of the lower part out of the apparatus without influencing the combustion zone. In a vertical tube the exhaust is separated from cooling water, condensed exhaust water and unburt fuel. Water is separated from the lighter fuel components through a siphon and drained off. The condensed fuel is collected in the reservoir for disposal.

Chapter 3

Experiments

The experiments are carried out at atmospheric pressure and 294 K ambient air temperature. The fuel mass fraction, the temperature and the component of the flow velocity normal to the stagnation plane at the fuel boundary are represented by $Y_{F,1}$, T_1, and V_1, respectively. The oxygen mass fraction, the temperature and the component of the flow velocity normal to the stagnation plane at the oxidizer boundary are represented by $Y_{O2,2}$, T_2, and V_2, respectively.

The accuracy of the strain rate is $\pm 10\%$ of recorded value and that of the fuel mass fraction $\pm 3\%$ of recorded value. The experimental repeatability on reported strain rate is $\pm 5\%$ of recorded value [3, 4].

3.1 Experimental Procedure for Autoignition

The temperatures of autoignition and extinction depend on the states of the system, meaning the pressure p and a_2, $Y_{F,1}$, T_1, $Y_{O2,2}$, T_2. As the air used in the oxidizer stream is not being diluted, the oxygen mass fraction is $Y_{O2,2} = 0.233$. The fuel duct temperature is held in the region $T_1 = 460 \ (\pm 20)$ K. Two types of autoignition experiments are carried out, holding either the fuel mass fraction or the oxidizer strain rate constant. To ease the experimental procedure, these two

experiments are done in sequence for every fuel.

3.1.1   Autoignition at constant fuel mass fraction

In this experiments the fuel mass fraction is held constant at $Y_{F,1} = 0.4$ to analyse the dependency of the ignition temperature from the oxidizer strain rate. After the flow field has established, the temperature of the oxidizer stream is steadily increased until autoignition takes place. A valve on the operator panel is temporarly switched to change the flow in the oxidizer duct from air to nitrogen for quick extinction of the flame. The temperature of the oxidizer is lowered again and every point of autoignition is repeated at least twice. The experiments are done in several gears of the syringe pump, representing several fuel supply rates.

3.1.2   Autoignition at constant oxidizer strain rate

The oxidizer strain rate is held constant at $a_2 = 500 \ s^{-1}$ in these experiments to point out the ignition temperature in dependency of the fuel mass fraction. The procedure is similar as mentioned above.

3.2   Experimental Procedure for Extinction

For extinction the brass top with pure air is used, therefore the oxygen mass fraction is $Y_{O2,2} = 0.233$. The oxidizer is not heated, so the oxidizer stream has ambient temperature $T_2 = 293$ K. The fuel duct temperature is held again in the region $T_1 = 460 \ (\pm \ 20)$ K.

At a certain gear a flame is established with a blowtorch. The strain rate is increased until the flame extinguishes. The extinction is done for every fuel rate at least three times.

3.3 Tested Blends

As the ethanol content in fuel is commonly stated in percentage by volume, this is also done in this thesis. In the autoignition and extinction experiments blends of gasoline and surrogate with contents of 0 vol%, 20 vol%, 40 vol%, 60 vol%, 85 vol% and 100% ethanol were examined. The properties of the blends of UTG96 and ethanol can be seen in Table 3.1. Properties of surrogate an ethanol mixtures

Table 3.1: Properties of UTG96-ethanol blends. Volume percentage and density given for 298 K.

	UTG96	UTG96 -E20	UTG96 -E40	UTG96 -E60	UTG96 -E85	E100
UTG96 [vol%]	100	80	60	40	15	0
Ethanol [vol%]	0	20	40	60	85	100
Molecular Weigth [g/mol]	105	82.7	68.6	58.8	50.1	46.1
Density [kg/m^3]	0.741	0.751	0.761	0.770	0.783	0.790

are shown in Table 3.2.

Table 3.2: Properties of Surrogate/Ethanol blends. Volume percentage and density given for 298 K.

	Surrog.	Surrog. -E20	Surrog. -E40	Surrog. -E60	Surrog. -E85	E100
Surrogate [vol%]	100	80	60	40	15	0
Ethanol [vol%]	0	20	40	60	85	100
Molecular Weigth [g/mol]	103.24	81.7	67.9	58.4	49.9	46.1
Density [kg/m^3]	0.730	0.742	0.754	0.766	0.781	0.790

Chapter 4

Experimental Results

The following sections summarize the experimental results.

4.1 Autoignition

The temperatures of the oxidizer stream at autoignition are corrected for radiation loss.The symbols represent arithmetically averaged temperature measurements and strain rates. The curves are best-fit lines based on logarithmic equations.

A given fuel will autoignite at temperatures higher than the shown points of autoignition. Therefore its curve separates the figure into two regions. Above the curve autoignition will always take place, below the curve the flow is frozen.

Because of already stated reasons UTG-96 was used for comparing the results for surrogate. With experiments it was demonstrated that UTG-96 has similar behavior in autoignition and extinction as Gasoline91.

4.1.1   Autoignition at constant fuel mass fraction

Figure 4.1 shows the temperature of the oxidizer stream at autoignition for different blends of UTG-96 with ethanol. For a specific fuel an increase of the strain rates, accompanied by higher flow velocities, decreases the time for chemical reactions. As a result the fuel stream is harder to ignite and the needed temperature for autoignition increases. This is reasonable considering the exponential correlation between temperature and reaction rates. The logarithmic behavior of the autoignition temperature indicates a smaller gradient $dT_{2,I}/da_2$ at higher strain rates. Therefore the autoignition temperature is less sensitive to strain rate changes at higher strain rates.
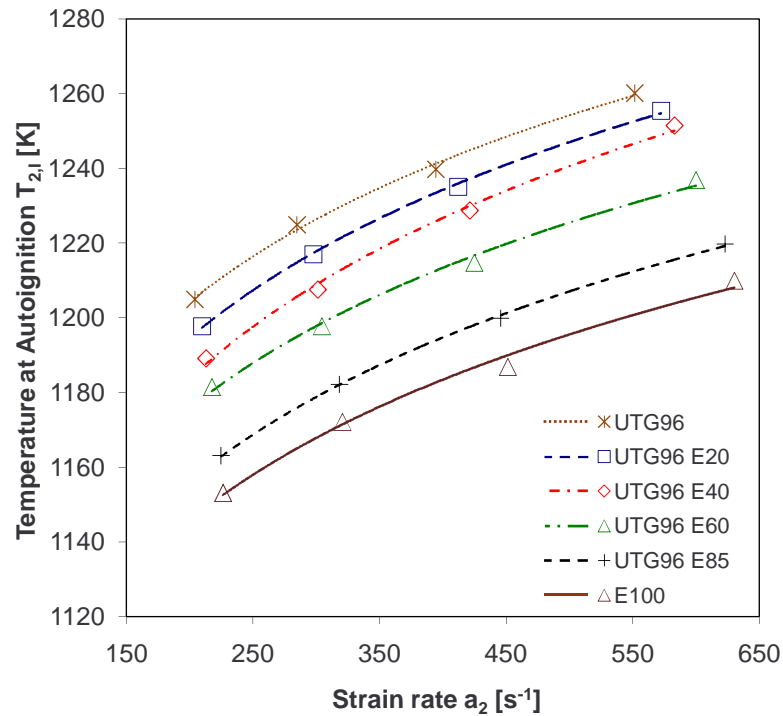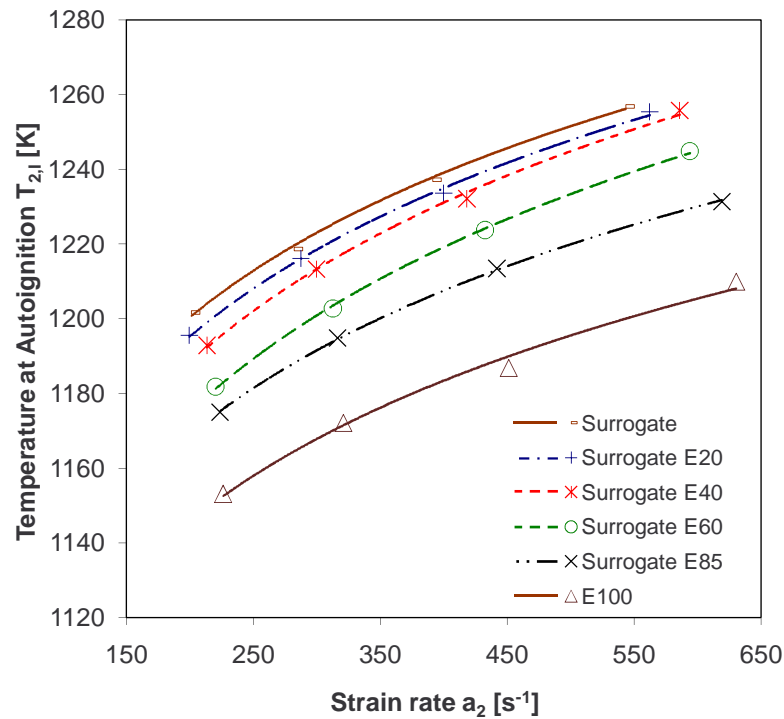

Figure 4.1: The temperature of the oxidizer stream at autoignition as a function of the strain rate at constant fuel mass fraction $Y_{F,1} = 0.4$. The figure shows data for blends of UTG96 and ethanol.

Ethanol is found to autoignite at lower temperatures than UTG-96. At first glance this seems to be conflicting to the octane rating, as ethanol has a higher knock resistance than gasoline. But, as already mentioned, the octane rating only repro-

duces the autoignition behaviour of a fuel in a defined CFR test engine at a certain speed and load. It does not paticularly account for the autoignition behaviour in diffusion flames at atmospheric pressure. In the range of $230\mathrm{s}^{-1}$ to $550\mathrm{s}^{-1}$ strain rate ethanol has a constantly ∼60K lower temperature at autoignition than pure UTG-96. It appears that ethanol mixed into UTG-96 has a uniform lowering effect on the autoignition temperature, independent of the strain rate.

Figure 4.2 displays the temperature of the oxidizer stream at autoignition for the

Figure 4.2: The temperature of the oxidizer stream at autoignition as a function of the strain rate at constant fuel mass fraction $Y_{F,1} = 0.4$. The figure shows data for blends of surrogate and ethanol.

blends of surrogate and ethanol. The same effect of ethanol on the temperature at autoignition was observed. Figure 4.3 compares the temperature of the oxidizer stream at autoignition for UTG96-ethanol blends and surrogate-ethanol blends.

It can be seen that over the hole range of strain rate pure surrogate is slightly easier to autoignite than UTG-96. This is consistent with results for this surrogate and commercial gasoline in a previous study [3]. For blends with ethanol the surrogate

tends to autoignite harder. With higher ethanol contents the difference gets bigger, resulting in a significant mismatch between UTG96 E85 and Surrogate E85.
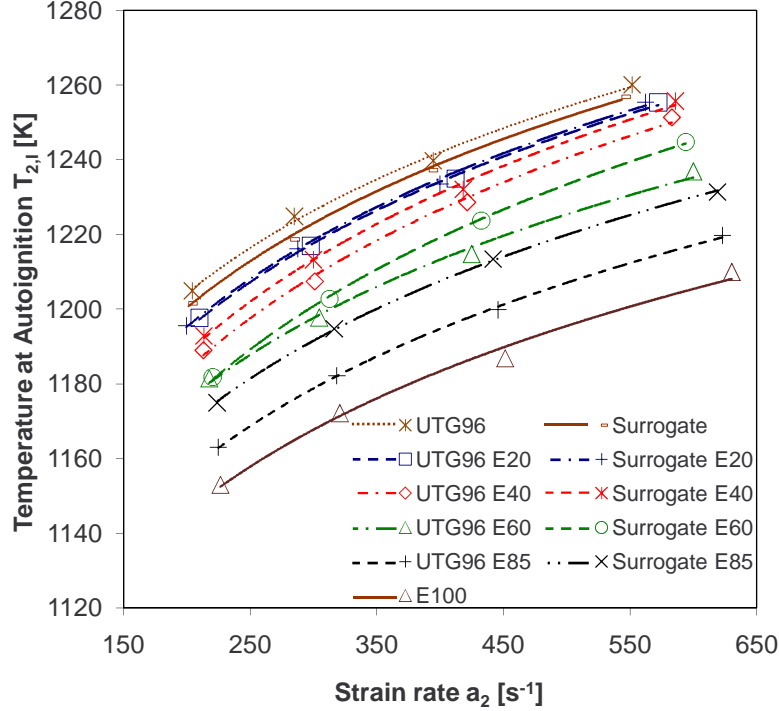

Figure 4.3: The temperature of the oxidizer stream at autoignition as a function of the strain rate at constant fuel mass fraction $Y_{F,1} = 0.4$. The figure shows data for blends of UTG-96 with ethanol and surrogate with ethanol.

Figure 4.4 shows the agreement of the surrogate-ethanol blends with UTG96-ethanol blends. On the left side the temperature of the oxidizer stream at autoignition for different blends of UTG-96 with ethanol and surrogate with ethanol over the ethanol content is shown. The points represent autoignition temperatures interpolated to $Y_{F,1} = 0.4$ and $a_2 = 500$ s^{-1}. The temperature of autoignition was gained from experiments at constant fuel mass fraction, interpolating along the logarithmic best fit curves. The lowering effect of ethanol in both blends can be seen, although it appears to have initially a stronger effect in blends with UTG-96. The right side displays the difference of said temperatures between UTG96-ethanol and surrogate-ethanol mixtures over ethanol content.

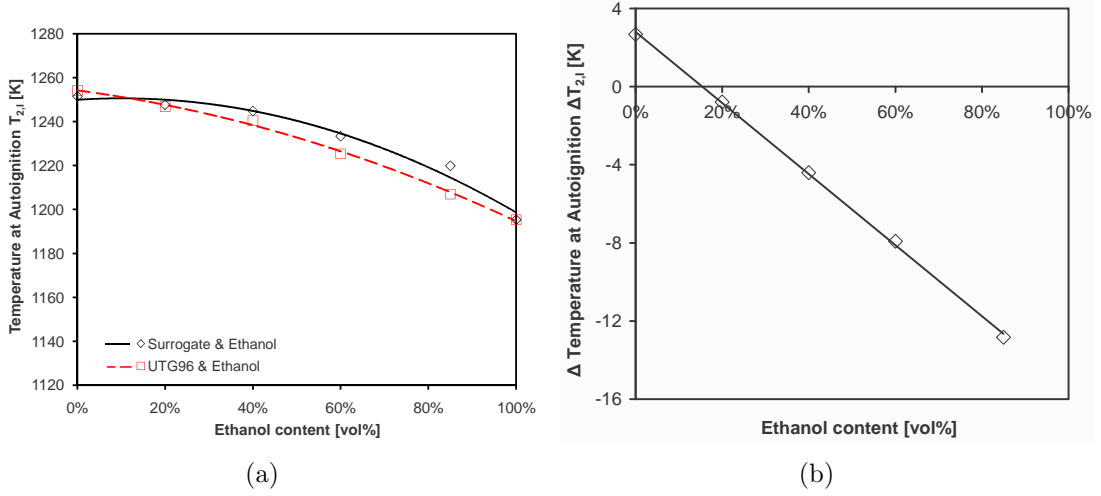It can be seen, that up to 40% of ethanol in the fuel, the UTG96-ethanol and

(a)

(b)

Figure 4.4: (a)The temperature of the oxidizer stream at autoignition as a function of the ethanol content for UTG96-ethanol and surrogate-ethanol blends. Data gained from experiments at constant fuel mass fraction $Y_{F,1} = 0.4$ by interpolation to constant oxidizer strain rate $a_2 = 500$ s^{-1}. (b)Difference between said temperatures of UTG96-ethanol and surrogate-ethanol blends.

surrogate-ethanol mixtures have a temperature of autoignition within a bandwidth of ± 4K. For this range the mixture of the surrogate and ethanol are considered to reproduce the autoignition behavior at constant fuel mass fraction for gasoline-ethanol blends. Surrogates with higher contents of ethanol do not reproduce this autoignition behavior apropriate.

Figure 4.5 shows the temperature of the oxidizer stream at autoigniton for UTG96-ethanol mixtures over the Research Octane Number. The temperature of autoignition was gained from experiments at constant fuel mass fraction by using the logarithmic best fit curve of the experiments. Octane numbers in blends of gasoline and ethanol do not obey a linear blending law, so the RON is approximated as a quadratic function over ethanol content. It is gained from the RON of pure fuel and pure ethanol and the effect on RON when blending small amounts of ethanol into gasoline.

Although ethanol serves as an octane enhancer, the temperature at autoignition decreases with higher ethanol content. The two component blend of n-heptane and iso-octane which defindes the octane numbers RON and MON do not have
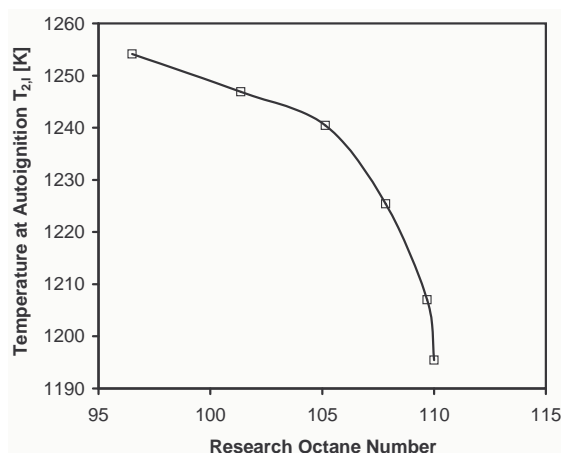
Figure 4.5: Temperature of the oxidizer stream at autoignition $T_{2,I}$ of UTG96-ethanol mixtures over RON. Temperatures gained from experiments at constant fuel mass fraction $Y_{F,1} = 0.4$ by interpolation to constant oxidizer strain rate $a_2 = 500$ s^{-1}.

not the ability of reproducing the autoignition behavior the figure would show a directly proportional relationship between RON and autoignition temperature.

4.1.2   Autoignition at constant oxidizer strain rate

Figure 4.6 shows the temperature of the oxidizer stream at autoignition for different blends of UTG-96 and ethanol for varying fuel mass fraction. A decrease of the fuel mass fraction, meaning a more dilluted fuel-nitrogen stream, leads to higher autoignition temperatures. This is reasonable, considering that the limit case of zero fuel in the fuel-nitrogen stream is not flammable and has therefore an infinitely high ignition temperature. The temperature follows a logarithmic dependency of the fuel mass fraction. An explanation is the linear relationship between concentrations and reaction rates.

Ethanol was found to have a uniform ~60K lower temperature at autoignition than pure UTG-96, similar to autoignition at constant fuel mass fraction. Blending ethanol into the gasoline caused over the full range of observed fuel mass fraction the same lowering effect, which can be seen in the parallel best fit curves. This indicates that UTG-96 and ethanol blends have a uniform mixing behavior over
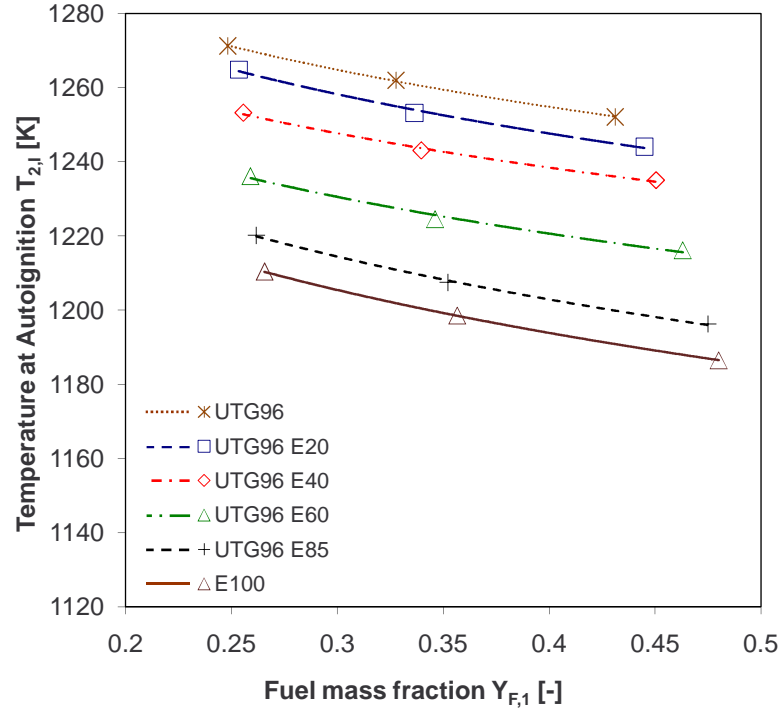
the fuel mass fraction.

Figure 4.6: The temperature of the oxidizer stream at autoignition as a function of the fuel mass fraction at constant strain rate $a_2 = 500 \ s^{-1}$. The figure shows data for blends of UTG96 and ethanol.

Figure 4.7 shows the temperature of the oxidizer stream at autoignition for the blends of surrogate and ethanol.

Figure 4.8 compares the temperature of the oxidizer stream at autoignition for blends of UTG-96 with ethanol and blends of surrogate and ethanol. Similar to experiments at constant fuel mass fraction pure surrogate appears to ignite slightly easier than UTG-96. A previous study [3] showed similar results for this surrogate and gas station gasoline. As seen in experiments at constant fuel mass fraction, with rising ethanol content surrogate-ethanol blends tend to become harder to ignite than UTG96-ethanol blends. The temperatures of the oxidizer stream at autoignition became more mismatching with higher ethanol contents. The Surrogate E20 blend reproduced the autoignition behavior of UTG96 E20 decent, whereas the Surrogate E40 showed similar behavior as UTG96 E40 only for fuel
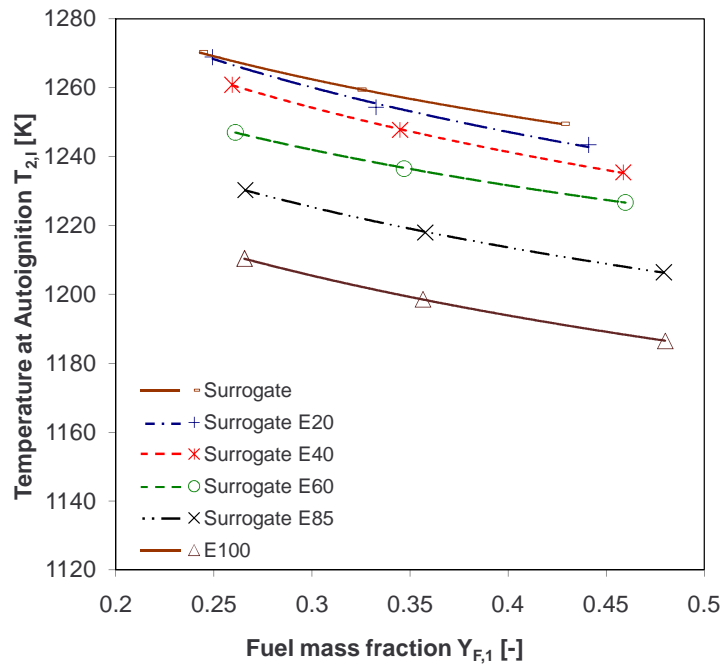
Figure 4.7: The temperature of the oxidizer stream at autoignition as a function of the fuel mass fraction at constant strain rate $a_2 = 500 \ s^{-1}$. The figure shows data for blends of surrogate and ethanol.
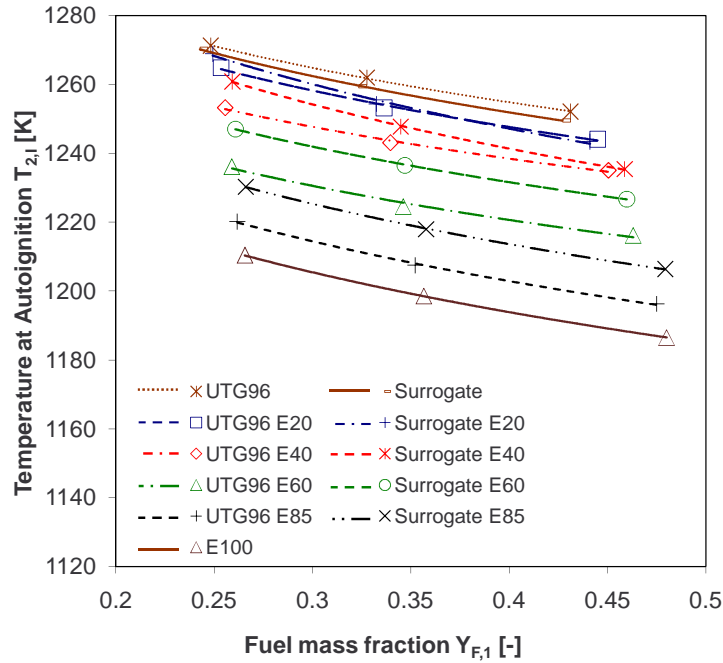

Figure 4.8: The temperature of the oxidizer stream at autoignition as a function of the fuel mass fraction at constant strain rate $a_2 = 500 \ s^{-1}$. The figure shows data for blends of UTG96 and ethanol.

mass fractions higher than 0.3.

4.2 Extinction

In experiments the similar extinction behavior of UTG-96 and Gasoline91 was demonstrated.

Figure 4.9 shows the result of extinction experiments for blends of UTG-96 and ethanol. The symbols denote arithmetically averaged fuel mass fractions over the oxidizer strain rates. The curves are best-fit lines.
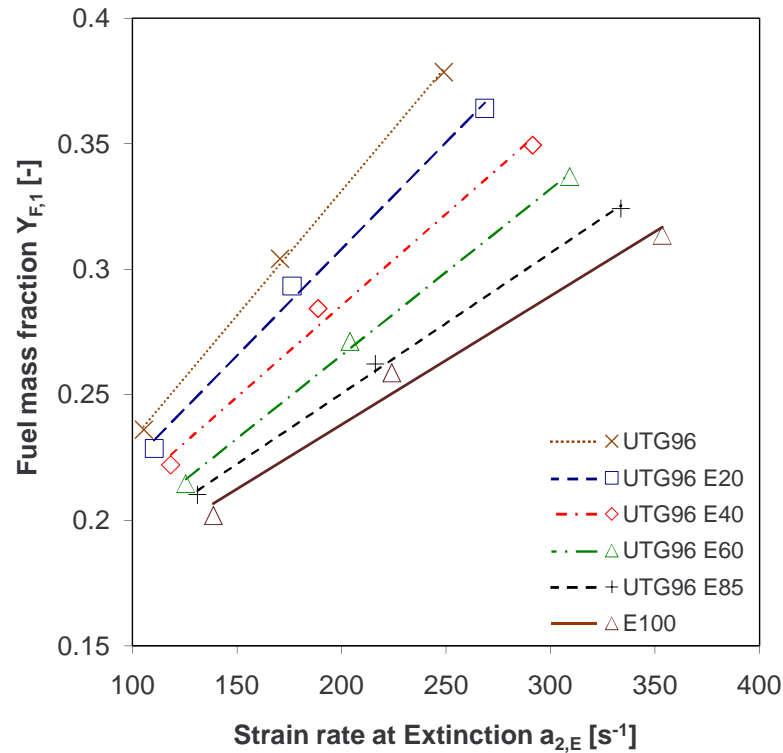

Figure 4.9: The fuel mass fraction as a function of the strain rate at extinction. The figure shows data for blends of UTG96 and ethanol.

A stabilized flame will extinguish at higher strain rates or lower fuel mass fractions than the shown points. Therefore the line is a boundary between the nonflammable and the flammable region. In a system in a state below the line a flame can not be ignited with an external energy source and stabilized. The flammable region can

be reached by either decreasing the strain rate, which results in a horizontal shift to the left, or increasing the fuel mass fraction, which equals an upward shift.

Ethanol was found to be more difficult to extinguish, meaning extinction occurs either at higher strain rates or at lower fuel mass fractions.

Figure 4.10 shows the fuel mass fraction as a function of the strain rate at extinction for blends of surrogate and ethanol. A similar behavior of the surrogate-ethanol
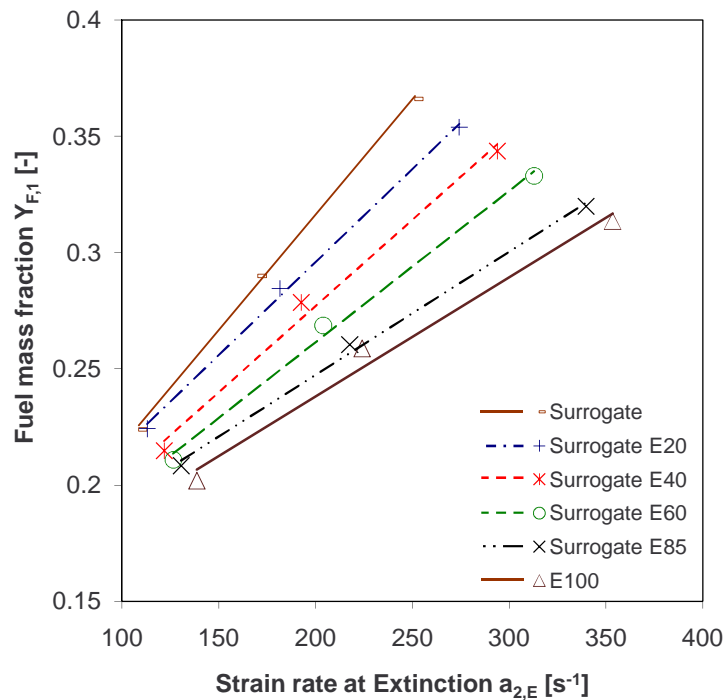

Figure 4.10: The fuel mass fraction as a function of the strain rate at extinction. The figure shows data for blends of Surrogate and ethanol.

blends was observed. Figure 4.11 compares the extinction behavior of UTG96-ethanol blends and surrogate-ethanol blends.

For any ethanol concentration and fuel mass fraction, the surrogate-ethanol blend is slightly harder to extinguish than the UTG96-ethanol blend. The agreement for pure UTG-96 and pure surrogate is adequate and gets better for higher ethanol content blends.

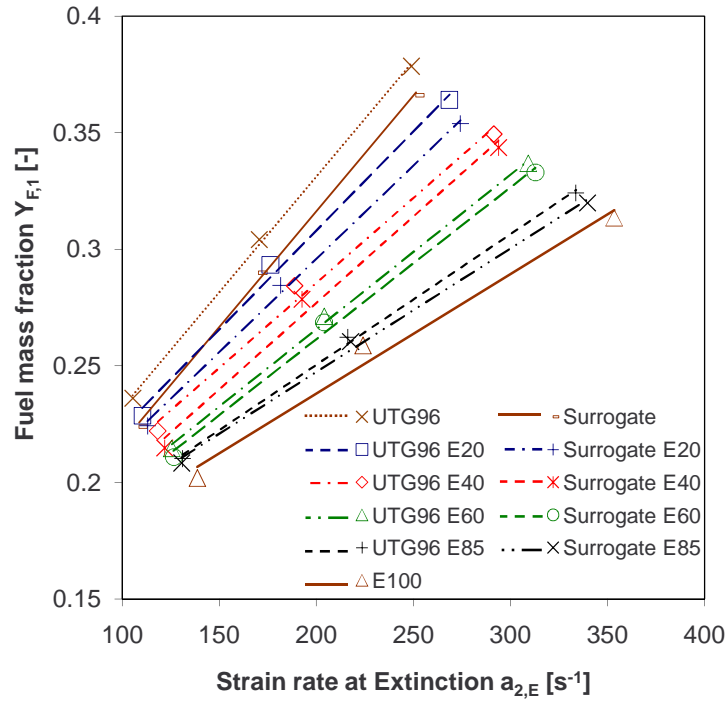The agreement of the surrogate-ethanol blends with UTG96-ethanol blends is

Figure 4.11: The fuel mass fraction as a function of the strain rate at extinction. The figure shows data for blends of UTG-96 with ethanol and surrogate with ethanol.

shown in Figure 4.12. On the right side the fuel mass fraction for different blends of UTG-96 and ethanol and surrogate with ethanol over the ethanol content is drawn. The points represent fuel mass fractions at a strain rate of $a_2 = 200 \ \text{s}^{-1}$ on the best fit curves of the experiments.
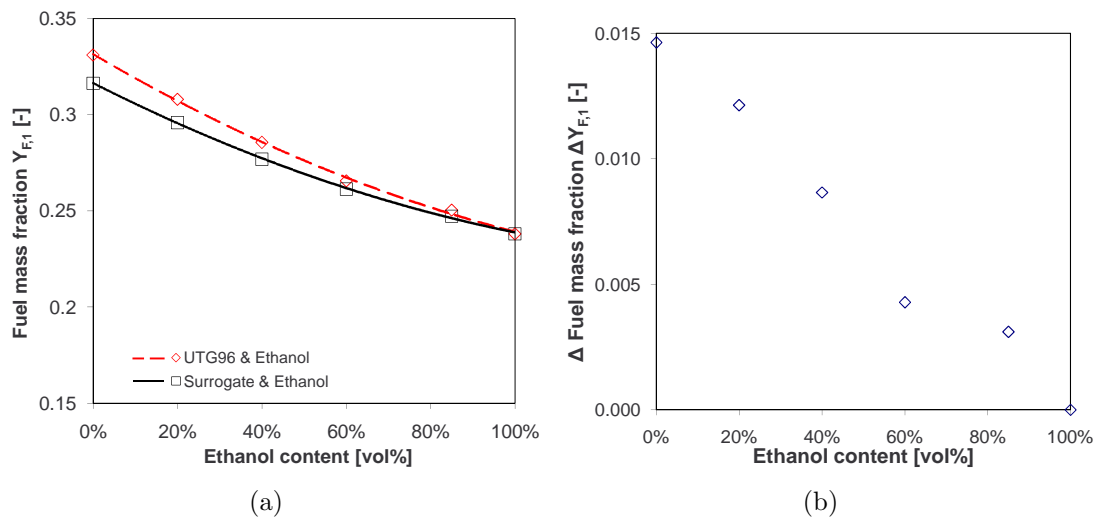
Figure 4.12: (a)The fuel mass fraction as a function of the ethanol content for UTG96-ethanol and surrogate-ethanol blends. Data gained from experimental data using the linear best fit lines and a strain rate of $a_2 = 200 \text{ s}^{-1}$. (b)Difference between UTG96-ethanol and surrogate-ethanol blends for said fuel mass fractions.

Chapter 5

Conclusion

In autoignition experiments ethanol was found to have a different influence on the temperature of autoignition in blends with UTG-96 and surrogate. This indicates that there are different interactions between surrogate and ethanol and UTG-96 and ethanol. Nevertheless blends of surrogate and ethanol have been found to reproduce the autoignition behavior of gasoline-ethanol mixtures with a ethanol content of up to 40 vol%.

The lowering effect of ethanol on the autoignition temperature is very remarkable. A previous study on burning velocities of ethanol-isooctane blends [6] pointed out a strong promotion of isooctane combustion by ethanol. The major intermediate species of ethanol during combustion is acetaldehyde CH_3CHO. It is the first oxidation stage of ethanol and plays a very important role in the combustion of hydrocarbons. A previous study [7] explored the influence of acetaldehyde and other aldehydes on hydrocarbon combustion. Acetaldehyde was found to promote the oxidation process at pre-flame stages and to lower the ignition temperature significantly.

The blends of surrogate and ethanol reproduced the extinction behavior of the corresponding blends of UTG-96 and ethanol wery well.

The surrogate in mixture with ethanol was proven to reproduce the autoignition

and extinction behavior up to a ethanol content of 40%.

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