B. TECH. PROJECT REPORT

On

Modelling Multicomponent Biodiesel Spray with Methyl Oleate and Methyl Laurate

BY

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DISCIPLINE OF MECHANICAL ENGINEERING

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Modelling Multicomponent Biodiesel Spray with Methyl Oleate and Methyl Laurate

A PROJECT REPORT

Submitted in partial fulfillment of the requirements for the award of the degrees

of
BACHELOR OF TECHNOLOGY
in

MECHANICAL ENGINEERING

Submitted by:
Aashish Sharma || 160003001

Guided by:
Dr. Devendra Deshmukh | Associate Professor

INDIAN INSTITUTE OF TECHNOLOGY INDORE
December, 2019

CANDIDATE'S DECLARATION

We hereby declare that the project entitled **"Modelling Multicomponent Biodiesel Spray with Methyl Oleate and Methyl Laurate"** submitted in partial fulfillment for the award of the degree of Bachelor of Technology in 'Mechanical Engineering' completed under the supervision of **Dr. Devendra Deshmukh, Associate Professor, Department of Mechanical Engineering,** IIT Indore is an authentic work.

Further, I declare that I have not submitted this work for the award of any other degree elsewhere.

Signature and name of the student(s) with date

Aashish Sharma

CERTIFICATE by BTP Guide(s)

It is certified that the above statement made by the students is correct to the best of my knowledge.

Signature of BTP Guide(s) with dates and their designation

Dr. Devendra Deshmukh

Associate professor

Preface

This report on "Modelling Multicomponent Biodiesel Spray with Methyl Oleate and Methyl Laurate" is prepared under the guidance of Dr. Devendra Deshmukh. Through this report, I have tried to give detailed analysis of Evaporating Spray Characteristics for bio-diesel mixtures of Methanol with Methyl Oleate and Methanol with Methyl Laurate through numerical simulations that I performed during my senior year at IIT Indore. While my work was preliminarily focused on numerical simulations, it can be carried forward in multiple dimensions in the future.

I have tried to provide all the details of the work that I have done so far for the reference of the students who wish to carry forward. I have tried my best to explain the content in lucid manner, whereas if some confusion persists feel free to reach out to me in that regard.

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I am immensely grateful to my supervisor Dr. Devendra Deshmukh for giving me an opportunity to do the B.tech Project under his guidance. His untiring patience towards correcting my mistakes and his faith in me for given tasks makes me complete the present work. I thank him for his invaluable guidance, suggestions, and encouragement throughout the work.

I would like to thank Mr. Vasudev Chaudhari, from Spray and Combustion Lab for helping me with the numerical solver for the simulations and providing me with technical guidance when and where required. I would like to thank Dr. Rajan Lanjekar from IISc Banglore, for providing valuable suggestions during the simulations. Without their kind support and help this work may not be possible.

Finally, I want to thank everyone who has, in one way or another, helped me to do this present work.

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Abstract

The biodiesel fueled CI engines are observed to produce higher NOx emission. The emissions depend on spray characteristic along with the composition and physiochemical properties of the biodiesel. The evaporating spray characteristics are analyzed using numerical models for biodiesel mixtures of methanol with methyl oleate and methanol with methyl laurate. The CFD code is modified to incorporate the physiochemical properties of the components of biodiesel mixtures and model multi-component evaporation.

The spray characteristics of evaporating spray, liquid length, and vapor length are computed. The spray tip penetration of karanja biodiesel is found to be similar to that of the methyl oleate. The spray tip penetration of coconut biodiesel is found to be similar to that of methyl laurate. So we can model these components of mixture as pure compound in the simulations.

The liquid length of methyl oleate's mixture is higher than methyl laurate's mixture. The liquid length also increases with decrease in the methanol ratio for both mixtures. The vapour length is hardly affected by the composition of the mixture. The in-cylinder temperature and pressure have obvious effect on the liquid length and also the vapour length. They increase with the rise in temperature and decrease with the rise in pressure. However the liquid length is more affected by the in-cylinder conditions.

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Chapter 1

Introduction

Compression Ignition (CI) engine exhibits higher thermal efficiency than that of spark ignition engines. This makes CI engine a popular choice for industrial, transport, and domestic power generation applications. The hazardous emissions, such as Particulate Matter (PM), Unburnt Hydrocarbon (UHC), Carbon Monoxide (CO) and Oxides of Nitrogen (NOx) which are the threat to human health and environment are the problems of CI engine. The CI engine fuel, diesel, is a fossil fuel having limited reserves all over the Globe.

The biodiesel is a renewable fuel for CI engine. Biodiesel gives similar engine performance as that of diesel with a lower PM and UHC emissions. However, higher NOx emission of biodiesel has become a major hurdle for its use in CI engines. Many numerical and experimental investigations are available in the literature analyzing the causes of higher NOx emission of biodiesel. The higher NOx emission of biodiesel is correlated to the fuel composition and properties. The dependence of emission on biodiesel composition motivates the researchers to find the optimal composition of biodiesel, which will have minimum engine emissions.

The advanced combustion technologies, to control NOx emission, such as Exhaust Gas Recirculation, multiple injection and Low Temperature Combustion strongly depend on air-fuel mixture formation. The air-fuel mixture formation depends on spray atomization and properties of fuel. It is important to understand an effect of the biodiesel composition on mixture formation through spray atomization and evaporation.

The combustion of the fuel is preceded by fuel evaporation and mixing with compressed air in the combustion chamber. The atomization of the injected fuel facilitates the vaporization of the fuel into fine droplets. Thus, the nature of atomized fuel governs the vaporization, mixture formation and hence combustion and nature of pollutants produced. The present study investigates role of composition of the fuel mixture and in-cylinder conditions on the atomization of fuel mixture under evaporating conditions. The air-fuel mixture formation is analyzed with multi-component evaporation models.

A literature study on the relationship between biodiesel properties and engine performance is presented in Chapter 2. A brief review of spray characteristics and their importance in combustion is discussed in this chapter. The numerical methodology used in this work is presented in Chapter 3. The evaporating spray characteristics at engine-relevant conditions for biodiesel mixtures used in this work are presented in Chapter 4. Finally, the conclusions and scope for future work is summarized in Chapter 5.

Chapter 2

Literature Review

The biodiesel, which is a renewable fuel, can be produced from oil from various sources, including edible and non-edible vegetable oils, waste oils, and fats. Transesterification is a widely used process for converting oils into biodiesels. The biodiesels are also termed as Fatty Acid Methyl Esters (FAMEs) or Fatty Acid Ethyl Esters (FAEEs), based on the alcohol moiety (methanol or ethanol) attached to the fatty acid chain. The Transesterification reaction for production of FAMEs from triglycerides is shown in the figure below.

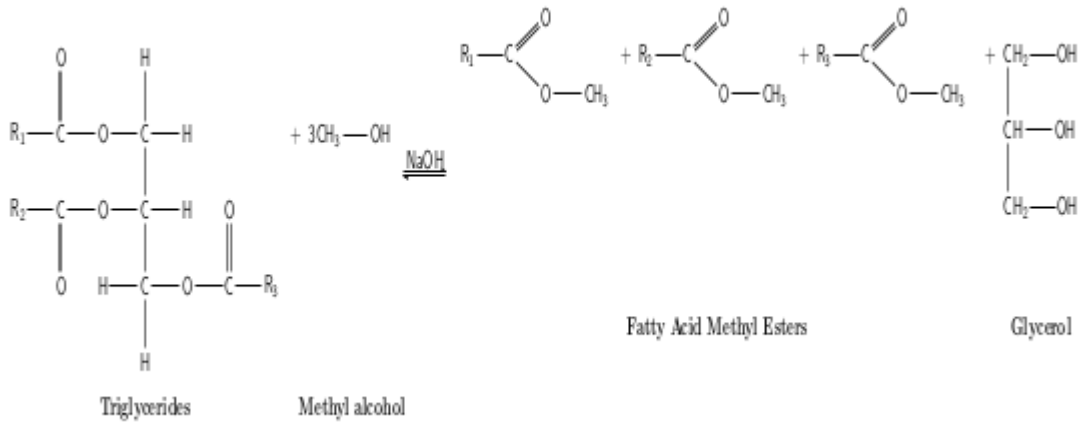

Figure 1:- Transesterification reaction

The Transesterification reaction replaces a heavy molecule of glycerol with a comparatively lighter molecular weight alcohol molecule, such as methanol or ethanol and produces mono-alcohol esters such as FAMEs or FAEEs.

Methyl oleate and methyl laurate are fatty acid methyl ester resulting from the formal condensation of the carboxy group with methanol. Methyl oleate and methyl laurate are prepared from oleic acid and lauric acid respectively. Both oleic acid and lauric acid are being produced in huge quantities from vegetable oils commercially and are major component in biodiesel. Kranja biodiesel can be approximated as methyl oleate for research purposes as it is the major component of kranja biodiesel. Similarly coconut biodiesel can be approximated as methyl laurate.

Biodiesels have a higher average boiling point (∼ 331 ◦ C) than that of diesel fuel (∼ 263 ◦ C). The energy density and lower heating value of biodiesel are less than that of diesel which is attributed to the presence of oxygen in biodiesel (around 10% by weight). Methanol on the other hand has a very low boiling point of 64.7 ◦ C. The energy density and lower heating value of methanol are way less than that of diesel which is attributed to the presence of oxygen in methanol (around 50% by weight).This significant difference of

normal boiling point among the components of the mixtures in terms of volatility differentials will exhibit different evaporating characteristics with varying ratio, which can be captured with multi-component evaporation model. Thus,there is a need to use multi-component evaporation model to study the vapor mass fraction of each individual species, which helps to improve the prediction of mixture formation, combustion characteristics, and nature of pollutants formed.

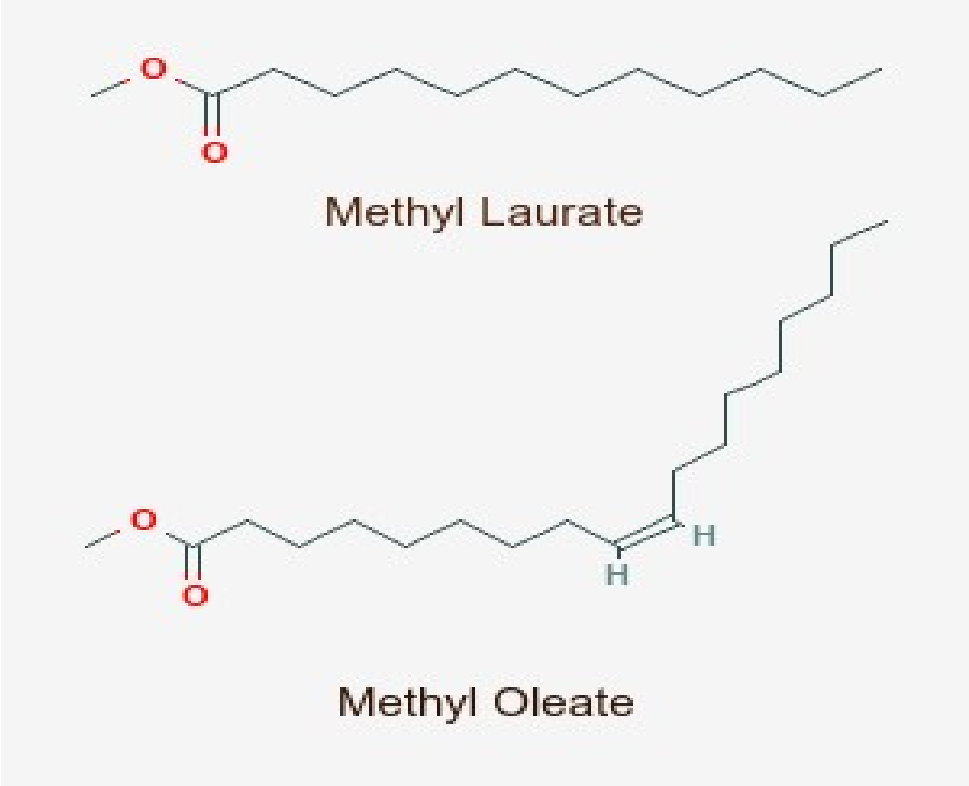

Figure 2:- Methyl Laurate and Methyl Oleate

The NOx emission in a typical diesel engine exhaust is composed of oxides of nitrogen with the major component being NO and lesser amount of NO2. High temperature (>1800 K) and mixture with equivalence ratio (<1) present at the periphery of diffusion flame are favorable conditions for thermal NOx formation. Additionally, a residence time of mixture at these conditions determine the amount of NOx formed. Therefore, any parameter or property which influences combustion temperature, equivalence ratio or residence time of air-fuel mixture can be responsible for NOx formation. So NOx emission with biodiesel as fuel can be controlled with advance in injection timing, combustion phasing and flame temperature.

The flame temperature can be reduced if the mixture is homogenized which is the basis of the Homogeneous Charge Compression Ignition (HCCI) technology. The combustion facing can be controlled if we could control the reactivity of the fuel. The fuel mixture with varying ratio is a smart way to control the reactivity of the fuel. And the charge with higher liquid length or vapour length approaches the homogeneous condition of HCCI technology.

Chapter 3

Methodology

A methodology to study the spray characteristics of biofuel mixtures is discussed in this chapter. The spray is modelled using OpenFOAM CFD code and its models. The code used is similar to the code used in the previous study of “Experimental and Numerical Spray Characterization of Biofuels and Pure Components” by Dr. Rajan Lanjekar with some slight variations in the parameters of KH-RT model and Rosin Rammler distribution for the fuel mixtures used in this study.

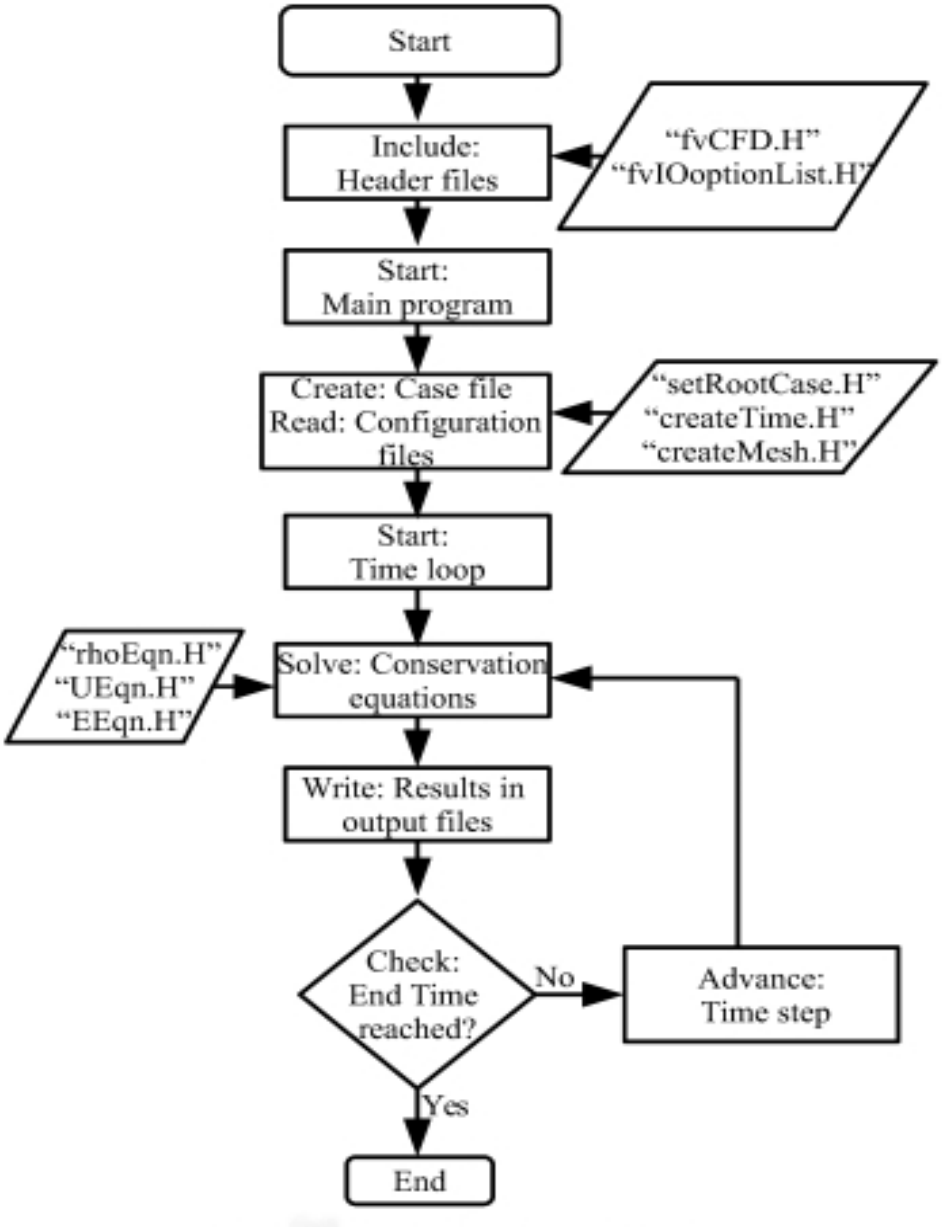

Figure 3:- Flowchart of a OpenFOAM solver

OpenFOAM provides with a solver called sprayFoam. The solver more or less mimics the power stroke of a 4-stroke engine. The combustion chamber geometry is a simple cuboid with dimensions of 100mm*30mm*30mm. It also provide with a injector which can be modified accordingly. It is a transient solver for compressible, turbulent flow with a spray particle cloud. The spray particle cloud is modeled with Lagrangian particle tracking option while combustion chamber is modeled with Eulerian approach. The mesh size is 1 mm along the height of the vessel, 0.5 mm along the width of the cuboid.

The time-step of 2.5 μs is used for the simulations. The fuel injector has an orifice diameter of 130 μm with a discharge coefficient of 0.9. is positioned at a distance of 0.5 mm below the top of the cuboid directed downwards along the central axis. The thermodynamic and physiochemical properties required for the implementation of the pure components are obtained from NSRDS functions and NASA Polynomials. Flow rate profile is generated with online website https://www.cmt.upv.es/ecn03.aspx.

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C13H26O2          T 6/09C 13.H 26.O  2.   0.G   298.150  5000.000 1000.        1
 3.03081525E+01 7.96191517E-02-3.11051295E-05 5.56126056E-09-3.73685618E-13    2
-9.05081000E+04-1.22080727E+02 5.61936131E+00 1.05866737E-01 3.73366256E-05    3
-1.19493586E-07 5.45578860E-11-8.14796222E+04 1.58696761E+01-7.49792832E+04    4

C19H36O2          T02/08C 19.H 36.O  2.   0.G   298.150  5000.000 1000.        1
 4.07415701E+01 1.13136819E-01-4.42917233E-05 7.92639065E-09-5.32644783E-13    2
-9.53175164E+04-1.61245167E+02 1.03900764E+00 1.89498279E-01-4.90208730E-05    3
-6.24648752E-08 3.76956066E-11-8.22671346E+04 5.24855188E+01-7.40734932E+04    4
```

NASA polynomials coefficients for methyl laurate (C13H26O2) and methyl oleate (C19H36O2)

Due to the various fuel ratio used in the simulations, the tuned parameters are not constant but are different for the different ratio. In the present study, the Rosin Rammler Diameters are varied as follow; Dmax[μm] is varied from Dmax = 300 to Dmax = 600 and average initial diameter D[μm] is varied from D = 132 to D = 378. For KH-RT model B0 = 0.61, B1 = 60, Ctau is varied from Ctau = 1 to Ctau = 40 and CRT is varied from CRT = 0.1 to CRT = 10.

The fuel is injected at an injection pressure of 1500 bar for 0.7 ms. Simulations are run for various combinations of pressure, temperature and mixture ratio. The combustion and chemistry modules of the code are turned off to study the spray under non reacting conditions.

Evaporating spray characteristics

The evaporating spray characteristics of biodiesel mixtures is presented in this chapter. The spray are studied at engine-relevant conditions such as late-cycle post-injection and near top-dead-center injection conditions. The spray characteristics liquid length and vapour length are predicted using the validated spray model.

4.1 Liquid Length

Liquid length is taken as the point unto which 95% of the liquid mass has reached.

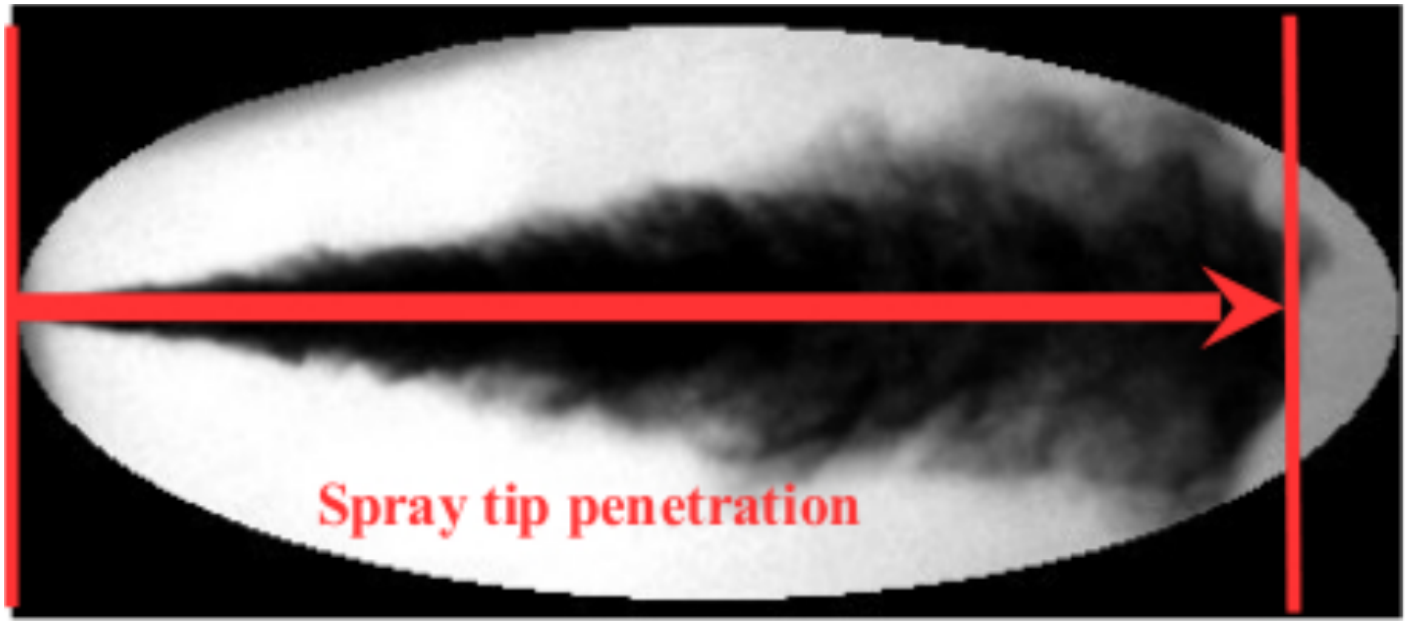

Figure 4:- Spray tip penetration

4.1.1 Effect of temperature

Simulations were carried out for two mixtures, one with 70% methanol and 30% methyl laurate, another one with 70% methanol and 30% methyl oleate. The back pressure in the in-cylinder was kept 30 bar constant and temperature was varied between 600 K to 900 K. As expected the liquid length increased with increase in temperature. The liquid length was between 46mm to 52mm, at a time 700 micro seconds after the start of injection gradually increasing with temperature. The liquid length of methyl oleate's mixture was slightly higher than that of methyl laurate's mixture.

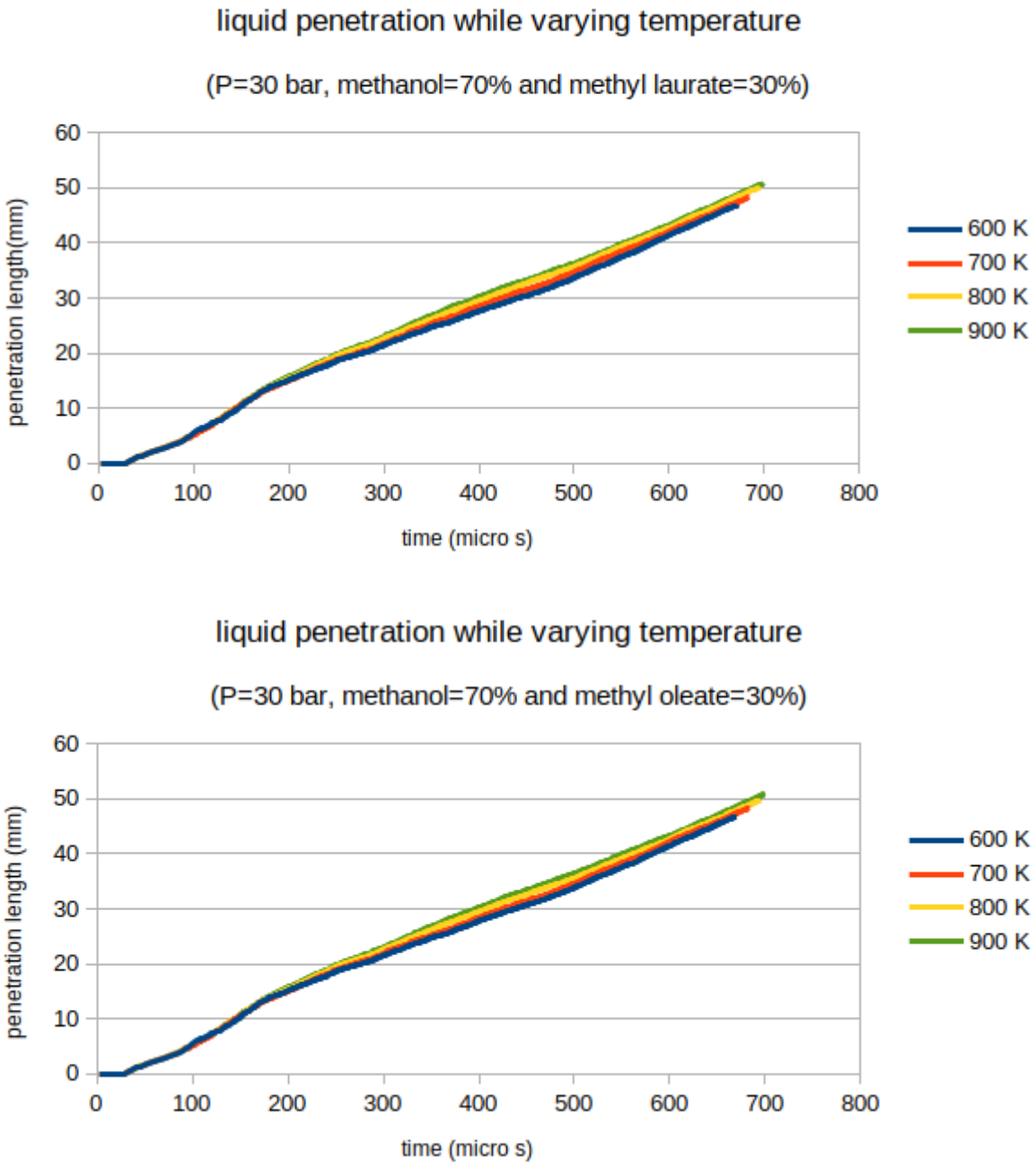

Figure 5:- Liquid penetration while varying temperature

4.1.2 Effect of pressure

Simulations were carried out for two mixtures, one with 70% methanol and 30% methyl laurate, another one with 70% methanol and 30% methyl oleate. The temperature in the in-cylinder was kept 800 K constant and back pressure was varied between 10 bar to 40 bar. As expected the liquid length increased with decrease in back pressure. The liquid length was between 45mm to 70mm, at a time 700 micro seconds after the start of injection gradually increasing with temperature. The liquid length of methyl oleate's mixture was slightly higher than that of methyl laurate's mixture.

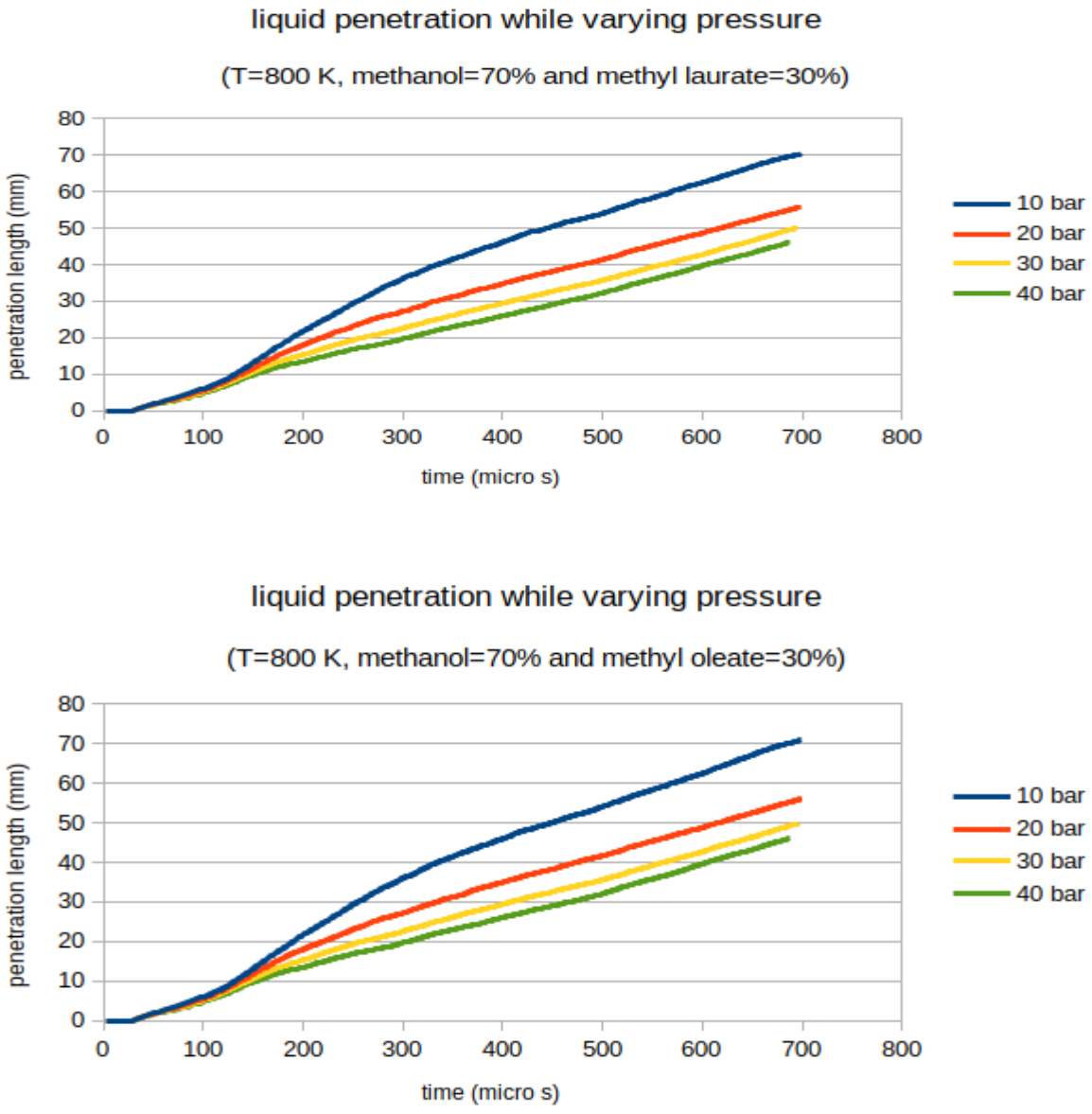

Figure 6:- Liquid penetration while varying pressure

4.1.2 Effect of methanol's ratio in the fuel mixture

Simulations were carried out for two mixtures, one of methyl laurate with methanol, another one of methyl oleate with methanol, while varying the methanol percentage from 60% to 80%. The temperature in the in-cylinder was kept 800 K constant and back pressure was kept 30 bar constant. The liquid length increased very slightly with decrease in methanol percentage of mixture, visible only after zooming in. The liquid length was around 26 mm, at a time 350 micro seconds after the start of injection and 46 mm, at a time 700 micro seconds after the start of injection gradually increasing with temperature. The liquid length of methyl oleate's mixture was slightly higher than that of methyl laurate's mixture.

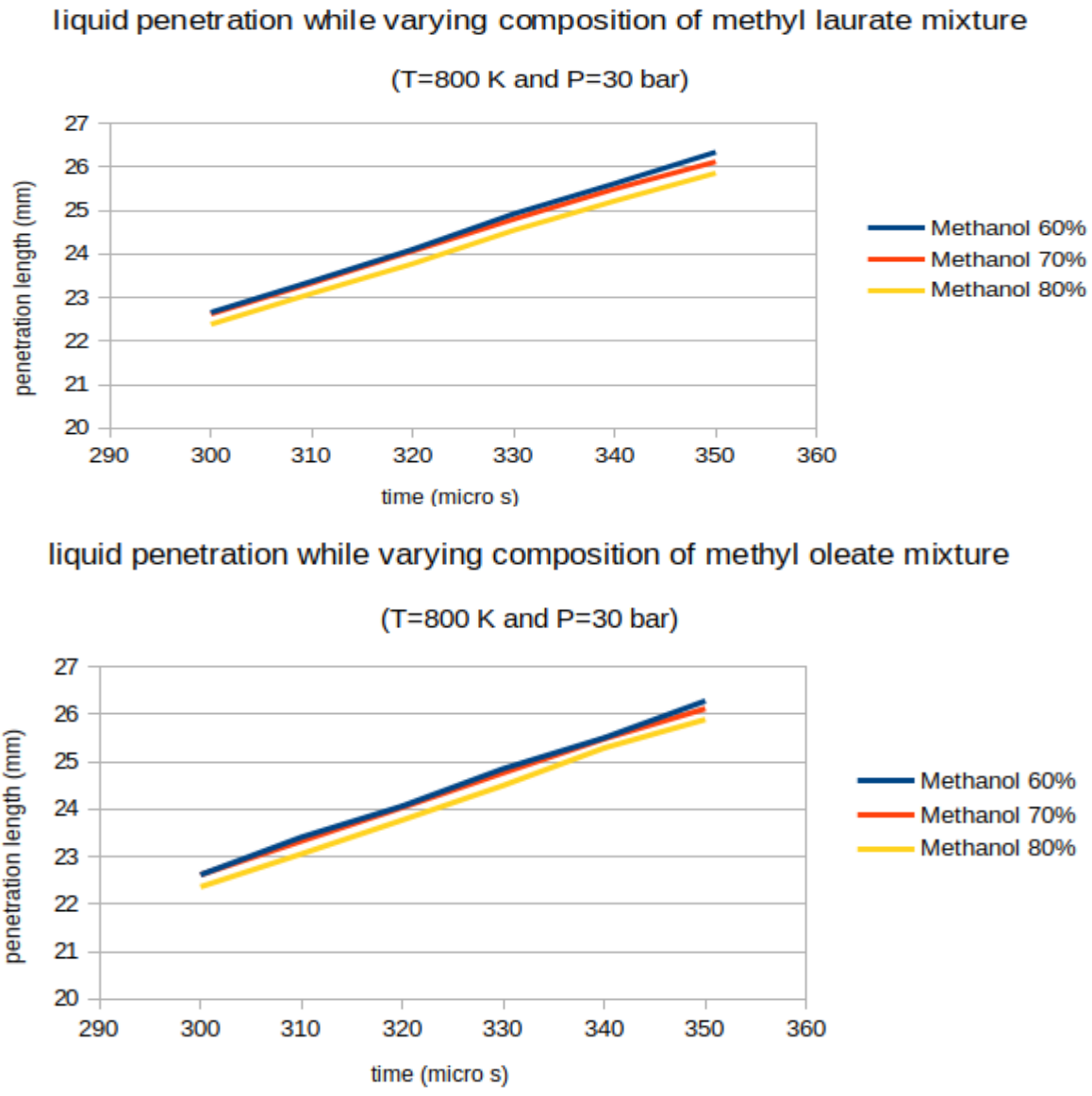

Figure 7:- Liquid penetration while varying ratio of fuel mixture

4.2 Vapour Length

For vapour length the bottom most point of contour of 1 % vapour mass fraction.

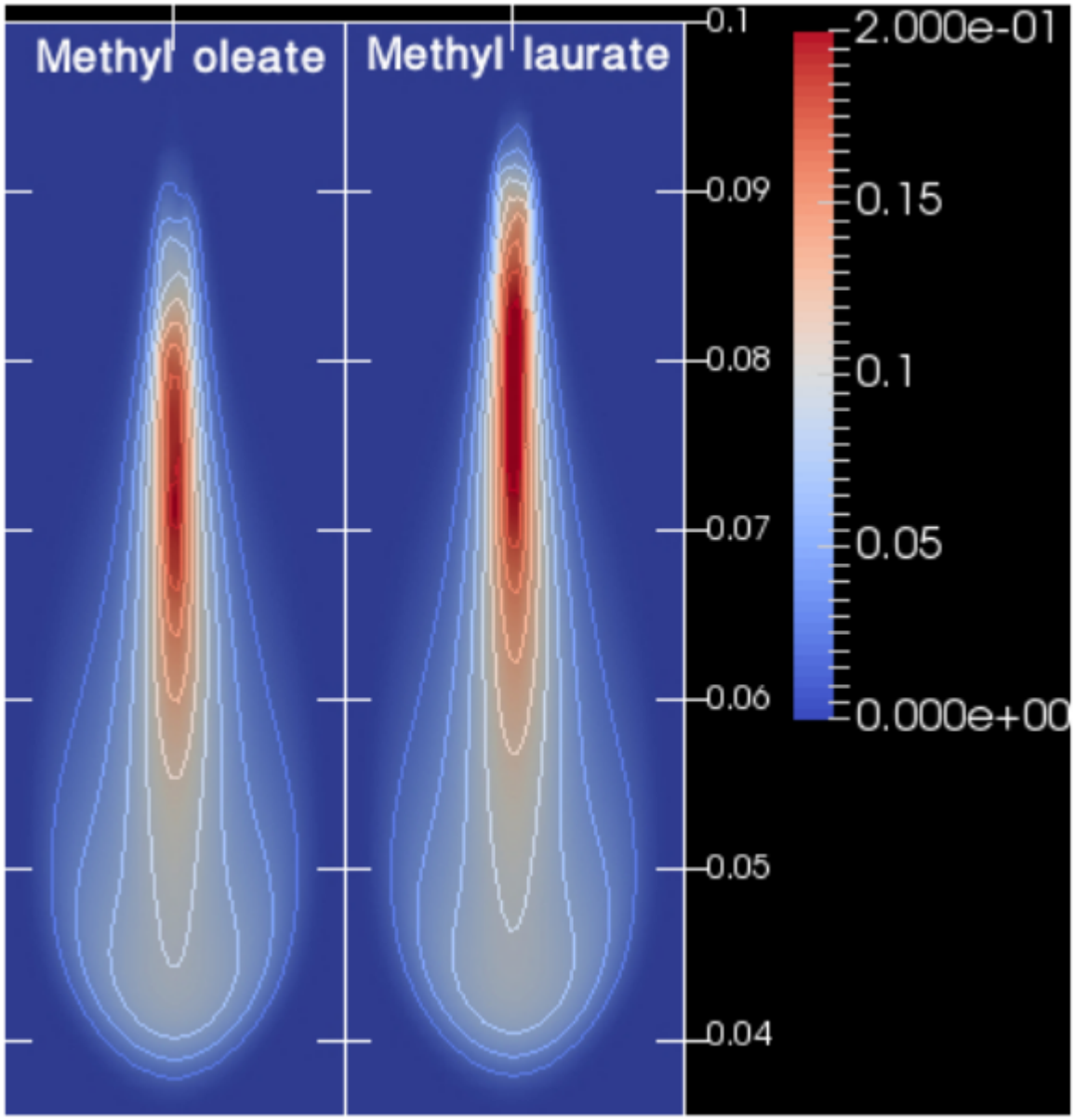

Figure 8:- Image of spray showing contours of vapour penetration of methyl laurate and methyl oleate

4.2.1 Effect of temperature

Simulations were carried out for two mixtures, one with 70% methanol and 30% methyl laurate, another one with 70% methanol and 30% methyl oleate. The back pressure in the in-cylinder was kept 20 bar constant and temperature was varied between 600 K to 900 K. However the vapour length was almost unaffected by the mixture's composition and ratio. Both mixtures gave approximately same results. As expected the vapour length increased with increase in temperature. The vapour length was between 93mm to 96mm, at a time 350 micro seconds after the start of injection gradually increasing with temperature.

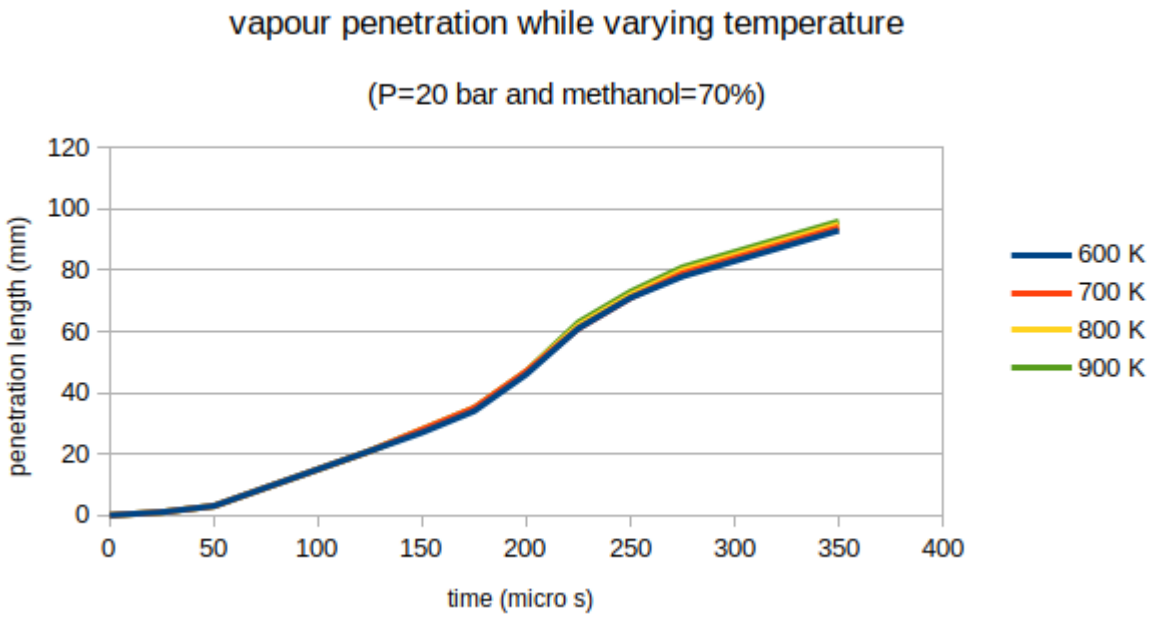

Figure 9:- Vapour penetration while varying temperature

4.2.2 Effect of pressure

Simulations were carried out for two mixtures, one with 70% methanol and 30% methyl laurate, another one with 70% methanol and 30% methyl oleate. The temperature in the in-cylinder was kept 800 K constant and the back pressure was varied between 10 bar to 40 bar. Similar to the previous case,one with the effect of temperature variation, the vapour length was almost unaffected by the mixture's composition and ratio. Both mixtures gave approximately same results. As expected the vapour length increased with increase in temperature. The vapour length was between 87mm to 96mm, at a time 350 micro seconds after the start of injection gradually increasing with temperature.

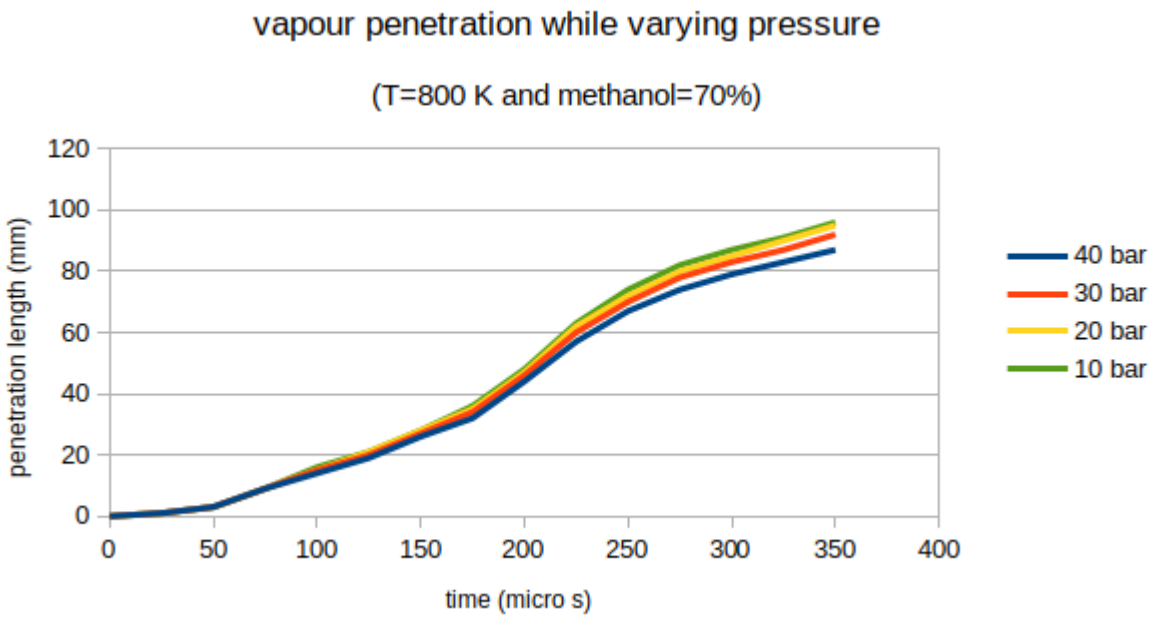

Figure 10:- Vapour penetration while varying pressure

Chapter 5

Conclusions and Future Work

The liquid length from an injector for fuel mixtures is a compounding effect of their density and volatility. The heavy (less volatile) fuel mixture produces less vaporized phase, thus its liquid length is greater than that of the lighter mixture. So because of methyl oleate being heavy and less volatile than methyl laurate, the methanol mixture with methyl oleate causes higher liquid length than the methanol mixture with methyl laurate. The liquid length increased with decrease in methanol percentage of mixture. However, the vapor penetration length is not that much influenced by the fuel type. In-cylinder temperature and pressure have expected effect on liquid length and vapour length. Both increases with increase in temperature and decrease in pressure.

The results produced here can be validated by experiments with the mentioned fuel mixtures. After that these results could be useful for combustion phasing and temperature control inside an engine. It will help in reducing the harmful emissions from vehicles. Emission control is necessary these days due to strict government policies and climate change.

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2. http://garfield.chem.elte.hu/Burcat/THERM.DAT , NASA Polynomials for thermodynamic and transport properties of individual species.
3. https://www.cmt.upv.es/ecn03.aspx , Flow rate profile generator.