ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE ENGINEERING AND TECHNOLOGY

INVESTIGATION OF RCCI ENGINE EMISSION AND PERFORMANCE

M.Sc. THESIS

Elif GÖZEN

Department of Mechanical Engineering

Automotive Programme

Thesis Advisor: Prof. Dr. Cem SORUSBAY

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

RCCI MOTORLARININ EMISYON VE PERFORMANS KARAKTERİNİN İNCELENMESİ

YÜKSEK LİSANS TEZİ

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MAYIS 2015

Elif GÖZEN, **a M.Sc.** student of **ITU Graduate School of Science Engineering and Technology** student ID 503121704, successfully defended the **thesis** entitled **"INVESTIGATION OF RCCI ENGINE PERFORMANCE AND EMISSIONS"**, which she prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

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To my family,

FOREWORD

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May 2015

Elif GÖZEN
(Mechanical Engineer, FORD OTOSAN)

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ABBREVIATIONS

ABDC	**:** After Bottom Death Center
AHRR	**:** Apparent Heat Release Rate
ATDC	**:** After Top Death Center
BBDC	**:** Before Bottom Death Center
BDC	**:** Bottom Death Center
BTDC	**:** Before Top Death Center
CA	**:** Crank Angle
CFM	**:** Coherent Flamelet Model
c_m	**:** Mean piston velocity
CTM	**:** Caracteristic Timescale Model
DI	**:** Direct Injection
DOC	**:** Diesel Oxidation Catalyst
DPF	**:** Diesel Particulate Filter
EBU	**:** Eddy Break up Model
ECFM	**:** Extended Coherent Flamelet Model
ECU	**:** Electronic Control Unit
EGR	**:** Exhaust Gas Recirculation
EVC	**:** Exhaust Valve Close
EVO	**:** Exhaust Valve Open
GSM	**:** Groupement Scientifque Moteurs
HCCI	**:** Homogeneous Charge Compression Ignition
IVC	**:** Intake Valve Close
IVO	**:** Intake Valve Open
IC	**:** Internal Combustion
ICE	**:** Internal Combustion Engine
k	**:** Turbulance kinetic energy
LCV	**:** Lower Calorafic Value
LNT	**:** Lean NOx trap
LTC	**:** Low Temperature Combustion
n	**:** Engine speed
PCCI	**:** Premixed Charge Compression Ignition
PDF	**:** Probability Density Function
PM	**:** Particulate Matter
RCCI	**:** Reactivity Controlled Compression Ignition
RI	**:** Ringing Intensity
RON	**:** Research Octane Number
S	**:** Engine stroke
SCR	**:** Selective Catalytic Reduction
SOF	**:** Soluble Organic Fraction
SOI	**:** Start of Injection
TDC	**:** Top Death Center

u' **:** Flactuating velocity
λ **:** Excess air factor

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INVESTIGATION OF RCCI ENGINE PERFORMANCE AND EMISSIONS

SUMMARY

The vehicle manufacturers and research institutes are seeking for clean and high efficiency combustion engine due to the increasing demand for crude oil and environment problems in recent years. Although aftertreatment system is capable of reducing engine emissions to a low level, the limitation of these systems that cannot make full use of fuel restricts the improvement in fuel economy. Large amount of researches focus on the LTC (low temperature combustion) strategy, which can achieve both the reduction of emissions and the improvement of fuel economy. RCCI (reactivity controlled compression ignition) is one of the tool to achieve this strategy, which is investigated in this study. The reactivity stratification in RCCI combustion is achieved by utilization of the separate injection system with low-reactivity and high-reactivity fuel introduced into cylinder directly in different injection timing. By using multi-dimensional CFD (computational fluid dynamics) modelling, it could be researched with fast and inexpensive way.

In this study RCCI engine investigated with diesel and methanol fuels based on NO and soot emission outputs regarding various mixture mass fractions and different SOI timings with EGR variants. Ecotorq 9L 380PS diesel engine has been used as diesel base case to verify model. AVL Fire ESE Diesel program has been used to get computational results and it has been compared with diesel engine dyno meter results taken from FORD OTOSAN test laboratories.

RCCI engine has been studied on 32 different variants overall. These 32 run includes; different SOI timings of methanol between 700-740 degree CA, different SOI timings of diesel between 704.8-714.8 degree CA, various EGR rates between %10 to %30, 7 different methanol mass fraction rated fuel mixtures overall. At first step created AVL Fire diesel engine model has been verified with engine dyno meter test results. This validated model mesh cell size chosen from 5 mesh variant option, regarding sensitivity of pressure, temperature, accumulated heat release, NO mass fraction, soot mass fraction results in order to achieve mesh independency.

RCCI engine results reviewed to understand behaviour and characteristics of methanol-diesel fuelled RCCI engine emission and performance. During that study NO mass fraction, NO mass per kWh, soot mass fraction, soot mass per kWh, CO mass fraction, indicated power, mean in cylinder pressure, mean in cylinder temperature, NO and soot distribution over combustion chamber, mean mass, diesel mass fraction in cylinder, methanol mass fraction in cylinder have been investigated and results compared with base diesel case for improvement assessment.

First batch of cases done to see behaviour of RCCI engine per methanol mass fraction rate from 0.18 to 0.94, called as case 2 to case 8. To define different fuel mixtures, diesel total heat release taken and kept same for all cases and injected methanol mass amounts calculated regarding to put same calorie inside of combustion chamber. Regarding that, 7 cases have been studied with methanol mass fractions from 0.18 to 0.94. Same engine parameters and modified ECFM-3Z combustion model has been used for RCCI cases. Diesel fuel SOI has been kept as the same as in diesel base case, and methanol injected at TDC (top death centre).

According to results of mixture variants, NO emission showed decreasing trend per methanol mass fraction increase, but soot emission shows increasing trend in opposite way. Efficient mixtures regarding NO and soot emission side, investigated to improve SOI timing as next. Case 2 and case 3 investigated on various methanol SOI timings to decrease soot and NO. Because those two cases have more promising soot emission results rather than five cases. During that cases diesel SOI kept same to understand methanol SOI effect on RCCI engine emission. Results showed that in all methanol SOI variant cases, from 715 to 740 degree CA, NO emission reduced %10-38 from base diesel case. Furthermore in soot point of view, methanol SOI from 715 to 720 CA, significant soot reduction observed in %53-54 percentage level. Thus, case 2 which has 0.18 methanol mass fraction rate understood as efficient mixture rate to achieve NO and soot reduction. Case 3 methanol SOI variant results showed average %80 NO reduction, but from all SOI variant cases' soot results are very high above from base diesel case, which makes 0.45 methanol mass fraction rate insufficient to reduce emissions without EGR application.

After understanding RCCI engine behaviour on methanol mass fraction rate and methanol SOI timing, EGR mass fraction rate affect investigated. For that investigation case 2 and case 3 selected, hence they are lowest soot emission rated cases. Because EGR affect expected to decrease NO, but increase soot simultaneously. Case 2 results aligned that argument exactly. But case 3 showed decrease on soot with EGR application.

With the light of that studies on methanol mass fraction and SOI and EGR rate, advance SOI on diesel and methanol fuel investigated to reduce soot emission. Because with previous methods NO emission could be reduced in high rates, but soot emission decrease didn't show high reduction rates as NO. Regarding that case 2 and case 4 selected for study, hence they have lowest soot emission observed case are. Case 2 investigated with %15 EGR application to combine EGR and advance SOI together. Case 4, which has 0.58 methanol mass fraction rate, investigated for non-EGR application to see only SOI effect on emission. Results of case 2 and case 4 shows that, increasing advance of diesel SOI leads to increase on soot emission no matter which methanol mass fraction rated mixture used. For methanol SOI advance, it was understood that higher advance on methanol SOI help to decrease soot, but increase NO emission simultaneously. Keeping diesel SOI same and increase advance on methanol SOI could work for non-EGR applied cases to decrease soot emission. But combining EGR and advance SOI cause increase on soot due to fuel gathered in piston bowl and couldn't find enough air to be burned and creates increase on unburned HC which leads to increase on soot emission.

Regarding all cases, most problematic part was soot improvement. In 25 cases, NO emission reduced from base diesel case, but soot improvement only achieved in 6 cases.

Soot mass reduced cases from base diesel case (Case 1) reviewed. Regarding results; case 2 with 0.184 methanol mass fraction and case 3 with 0.45 methanol mass fraction are successful to achieve soot reduction. With all those cases NO emission reduction also achieved simultaneously. In 6 cases power decrease, which reaches up to %7 percentage, observed. NO and soot reduction percentages calculated from mass per kWh, hence power decrease also calculated and even that emission decrease observed.

According to priority best case could be selected. If soot reduction required to be lowest one, case 3.h can be selected, which has 714.8 diesel SOI, 715 methanol SOI, %10 EGR, 0.45 methanol mass fraction. That provides %80 percentage soot reduction and %4 NO reduction. If NO reduction required being lowest one, case 3.j can be selected, that has same attributes with increased EGR rate to 0.25. That provides %62 NO reduction with %51 soot reduction.

RCCI MOTORLARININ EMISYON VE PERFORMANS KARAKTERININ INCELENMESI

ÖZET

Son yıllardaki ham petrol kaynaklarına artan talepler ve çevre sorunları sebebiyle araç üreticileri ve araştırma enstitüleri, motorlarda temiz ve verimli yanma elde etme araştırmalarına yöneldiler. Aftertreatment sistemleri emisyon azaltılmasında başarılı olmasına rağmen, regülasyon limitlerinin tutturulması özellikle yakıt ekonomisinin sağlanmasında başarılı olamamakta. Araştırmaların büyük bir kısmı hem emisyonları düşürme hem de yakıt ekonomisni iyileştirme olanağı sağlayan, LTC stratejisine yoğunlaşmış durumda. RCCI motorları LTC stratejisinin kullanım alanlarından biri. RCCI motorlarının temel prensibi düşük ve yüksek reaktiviteli yakıtların farklı zamanlarda silindir içine ayrı enjektör sistemleriyle sağlanmasından oluşur. Bu konu çok yönlü CFD modellemenin kullanılmasıyla daha kısa sürede ve daha ucuz olarak araştırılabilir.

Bu çalışmada RCCI moturunda azotoksit ve partikül emisyonları, methanol ve dizel yakıtını farklı yakıt karışım oranları, farklı enjeksiyon zamanları ve bunlara EGR etkisi araştırılmıştır. Dizel motoru olarak Ecotorq 9L 380PS motoru kullanılmış olup, dizel modelinin doğrulanmasında kullanılmıştır. Dizel modelin doğrulanmasında FORD OTOSAN test labratuarlarından alınan motor dinamometre sonuçları ile AVL Fire CFD programının analiz sonuçları kullanılmıştır.

RCCI motoru 32 farklı analiz deneyi ile incelenmiştir. Bu 32 deney; 700-740 derece krank açısı arasında değişen metanol enjeksiyon zamanları, 704.8-714.8 derece krank açısı arasında değişen dizel enjeksiyon zamanları, yüzde 30 ile yüzde 10 arasında farklı EGR oranları ve 7 farklı metanol dizel karışım oranları ve birbirleriyle olan kombinasyonları sonucunda oluşturulmuştur. İlk olarak AVL Fire programında oluşturulan dizel modeli motor dinamometre sonuçları ile karşılaştırılmış ve doğrulanmıştır. Validasyonu tamamlanmış model için uygun mesh hücre boyutu seçimi 5 farklı seçenek arasından silindir içi ortalama basınç, sıcaklık, kümülatif ısı yayılımı, NO ve partikül madde kütlesel oranları karşılaştırılarak yapılmıştır.

Metanol ve diesel yakıtlarını kullanan RCCI motorunun emisyon ve performans açısından davranışlarını anlamak için model sonuçları incelenmiştir. Çalışma boyunca oluşan kütlece NO oranı, kWh başı NO kütle oluşumu, kütlece is oluşum oranı, kWh başına kütlece is oluşumu, CO kütle oluşum oranı, indike güç, ortalama silindir içi basınç ve sıcaklık, yanma odası içerisinde NO ve is dağılımı, ortalama hava kütlesi ve toplam kütle, zamana bağlı silindir içi dizel ve methanol kütle oranı değişimi sonuçları incelenmiş ve baz diesel modeli ile kıyaslanarak, parametrelerdeki değişim değerlendirilmiştir.

İlk çalışma RCCI motorunun 0.18 den 0.94 arası değişen metanol kütle oranına karşı davranışını gözlemlemek için yapılmıştır. Değişik karışım oranları seçilirken, dizel baz modeldeki ısı yayınımı alınmış ve RCCI deneyleri için sabit tutulup, enjekte edilen metanol oranı buna göre hesaplanmıştır. Buna göre 7 farklı karışım oranında deney üzerinde çalışılmıştır. Çalışmada aynı motor parametreleri dizel modelden alınmış ve ECFM-3Z yanma model parametreleri temelde aynı kalmak şartıyla çoklu yakıt kullanımı sebebiyle modifiye edilerek kullanılmıştır. Bütün karışım varyantları için dizel yakıtı püskürtme başlangıcı RCCI modelinde dizel baz model ile aynı alınmış, metanol ise üst ölü noktada püskürtmeye başlatılmıştır. Değişken karışım oranlı RCCI vaka sonuçlarına göre, methanol oranı arttıkça NO emisyonu azalma trandi gösterirken, is oluşumu artış göstermiştir. İs ve NO emisyonu bakımından en ideal sonuçlar, püskürtme başlangıç zamanlamasının iyileştirilmesi için üzerinde çalışılmıştır.

2. ve 3. vakalar bu çalışma için seçilmiş ve emisyonları azaltmak için farklı methanol püskürtme başlangıç zamanları araştırılmıştır. Çünkü bu iki vaka is emisyonu açısından diğer beş farklı vakaya göre çok daha iyi sonuçlar göstermiş, baz dizel vaka limitlerinin altında kalmışlardır. Metanol püskürtme başlangıcı değişiminin RCCI motorlarında emisyonunu anlamak adına deneyler boyunca dizel püskürtme zamanı sabit tutulmuştur. 715-740 krank açısı arası farklı metanol püskürtme başlangıçlı deney sonuçlarına göre, dizel baz vakası ile karşılaştırıldığında, NO emisyonu %10-38 arası azalma göstermiştir. Bunun yanında 715-720 krank açısı arasında yapılan püskürtme başlangıçları için is emisyonu açısından da %53-54 oranında azalma görülmüştür. Buna göre 0.18 metanol kütle oranlı 2 için NO ve is emisyonunu düşürmede başarılı bir karışım olduğu anlaşılmıştır. 3 nolu vaka için metanol püskürtme başlangıcı varyantlı deney sonuçları ise %80 oranında daha az NO emisyonu göstermiş, fakat bütün analizlerde dizel vakasına göre çok daha yüksek is oluşumu göstermiştir. Bu sonuçlar 0.45 metanol kütle oranlı case 3 karışımının EGR eklenmediği sürece emisyonu azaltmakta başarılı olmadığını ortaya koymuştur.

RCCI motorlarında metanol kütle oranı ve metanol püskürtme başlangıç zamanının anlaşılması sonrasında, EGR oranının etkisi araştırılmıştır. Bu çalışma için vaka 2 ve vaka 3 yakıt karışım oranları en düşük is oluşumunu gösteren vakalar olması sebebi ile seçilmiştir. Çünkü mevcut modellere EGR eklenmesi ile NO emisyonunun azaltılırken, is oluşumunu arttırulması beklenmektedir. Deney sonuçları vaka 2 nin bu argümanı destekler nitelikte olduğunu gösterirken, vaka 3 modeline EGR eklenmesi ile is oluşumunda azalma gözlenmiştir.

Değişken metanol kütle oranlı deney sonuçları, değişken metanol püskürtme başlangıcı zamanllı deney sonuçları ve farklı EGR oranlı deney sonuçlarından edinilen bilgiler ışığında, is oluşumunu azaltmak için, hem dizel hem de metanol pürkürtme zamanlarının erkene alınması üzerinde deneyler yapılmıştır. Çünkü yukarda bahsedilen metodlar ile NO emisyonunda yüksek oranlarda azalma sağlanırken, is oluşumu oranındaki azalmalar NO emisyonundaki gibi yüksek mertebelerde olmamıştır. Bu araştırma dahilinde vaka 2 ve vaka 4 en düşük soot emisyonlu vaka'ler olması sebebiyle seçilmiştir.

Vaka 2 karışımı %15 EGR ve erken püskürtme uygulanarak incelenmiştir. Vaka 4 ise EGRsız uygulamalarda erken püskürtmenin etkisinin anlaşılması için incelenmiştir. vaka 2 ve vaka 4 sonuçları, metanol yüzdesinin ne olursa olsun dizel yakıtı püskürtmesinin erkene alınmasının is oluşumunu arttırdığını göstermiştir. Metanol erken püskürtmesinin ise is oluşumunu azalttığı, fakat NO emisyonunu arttırdığını göstermiştir. Dizel püskürtme zamanının sabit tutulup, metanol püskürtme zamanının öne alınması EGRsız uygulamalarda is emisyonunu düşürmek için çözüm olabilir. Fakat EGR ve erken püskürtme stratejilerinin bir arada kullanılması, yakıtın enjeksiyon sonrası çanakta birikmesi ve yeterli hava bulamadığı için yanmamış hidrokarbonlara dönüşerek is emisyonunu arttırması sebebiyle önerilmemektedir.

Tüm çalışmalardan alınan sonuçlara göre is oluşumu azaltılmasında en büyük problem teşkil etmiştir. Koşulan analizlerden, 25'ünde NO emisyonunda azalma gözlenebilirken, sadece 6 tanesinde is oluşumu düşürülebilinmiştir.

İs oluşumunun dizel vaka (vaka1)'e göre azaltıldığı deneyler incelenmiştir. Buna göre, 0.18 metanol oranlı vaka 2 varyantları ve 0.45 metanol oranlı vaka 3 varyantları is oluşumunun azaltılmasında başarılı olmuştur. Bu vakalarda NO emisyonun da azaltılması sağlanmıştır. 6 vakada %7 oranında güç düşüşü gözlemlenmiştir. NO ve is azaltılma oranları kWh başına düşen emisyon kütlesine göre hesaplanmış olup, güç düşüleri ana karşılaştırma oranının içerisinde yer almaktadır.

Öncelik sırasına göre en iyi model seçilebilir. Eğer is oluşumu azaltılması esas alınıyorsa, vaka 3.h seçilebilir. Bu vaka 714.8 krank açısı dizel püskürtme başlangıcı, 715 krank açısı metanol püskürtme başlangıcı, kütlece %10 EGR, %45 metanol oranı içermektedir. Bu şekilde %80 oranında is oluşumunda, %4 oranında da NO azaltılabilir. Eğer NO emisyonu azaltılması esas alınırsa, vaka 3.j seçilebilir. Bu vaka de 3.h ile aynı olup, yalnızca EGR oranı %25'e çıkarılmıştır. Bu şekilde de %62 oranında NO emisyonunda azalma, %51 oranında is oluşumda azalma sağlanabileceği tespit edilmiştir.

1. INTRODUCTION

1.1 Purpose of Thesis

Clean and high efficiency combustion engine is taking attention in recent years due to the increasing demand for crude oil and environment problems by Automotiv Industrie. Even aftertreatment systems are capable of reducing engine emissions to a low level, as a result of regulation limitations, it is not possible to achieve limits only using those systems. Hence, combustion improvements of engine taking priority to get lower emission.

Diesel systems are much more efficient and preferable as compared with gasoline engines. Modern diesel engines have overcome disadvantages of earlier models of higher noise and maintenance costs. They are now quiet and require less maintenance as compared with gas engines of similar size. They are more rugged and reliable. There is no sparking as the fuel auto-ignites. The absence of spark plugs or spark wires lowers maintenance costs. Fuel cost per Kilowatt produced is thirty to fifty percent lower than that of gas engines. An 1800 rpm water cooled diesel unit operates for 12,000 to 30,000 hours before any major maintenance is necessary. An 1800 rpm water cooled gas unit usually operates for 6000-10,000 hours before it needs servicing. Gas units burn hotter than diesel units, and hence they have a significantly shorter life compared with diesel units. Furthermore diesel fuel is priced higher than gasoline, but diesel has a higher energy density, so more energy can be extracted from diesel as compared with the same volume of gasoline. Therefore, diesel engines in automobiles provide higher mileage, making it an obvious choice for heavy-duty transportation and equipment. Diesel is heavier and oilier compared with gasoline, and has a boiling point higher than that of water. And diesel engines are attracting greater attention due to higher efficiency and cost effectiveness.

In overall diesel engine is most preferable option even disadvantages. To overcome diesel engine problems, mainly NO and soot emission, RCCI engine strategy targeted with methanol and diesel fuels in separate injection method in number of methanol mass fraction rated mixtures, to be used as a part of LTC strategy, which is much more successful to control ignition and low pressure rise rate rather than PCCI or HCCI engines, even with keeping emissions low and fuel efficiency higher. With this methodology NO and soot reduction expected to be achieved regarding literature research. Researchs shows that LTC has great affect on reduction of emissions and the improvement of fuel economy in the same time.

LTC strategy can be achieved by using HCCI (Homogeneous charge compression ignition) or PCCI (Premixed charge compression ignition) or RCCI (Reactivity controlled compression ignition). RCCI is much more successful to control ignition and low pressure rise rate rather than PCCI or HCCI, even with keeping emissions low and fuel efficiency higher.

RCCI combustion strategy has been achieved by using separate injection systems for different fuel types, which has different reactivity attributes from each other, on different injection timings into cylinder directly.

In this thesis, RCCI strategy focused on using methanol and diesel fuel injections in different timings with various affect to achieve decrease on NO and soot mass without decrease on engine power.

It is clear that optimization on many operating parameters required to achieve better performance in RCCI engine strategy. To decrease research time and costs, numerical testing method is becoming biggest competitor rather than conventional experimental tests. AVL Fire software provides opportunity to establish model and fulfill combustion optimization ideas with gaining benefits of decreasing expenses and time.

1.2 Literature Review

In this thesis, 6 articles 3 lessons note has been studied.

Gong investigated methanol as an alternative fuel to cope with the shortage of energy sources in spark-ignition engines [1]. But for methanol usage in diesel applications not fully comprehend yet. In regulation perspective, methanol is environment friendly fuel with including oxygen atom in its molecule.

Reduction of NOx (nitrogen oxide) formation can be achieved by decreasing combustion temperature, on account of latent heat of vaporization of methanol. Moreover reactivity difference between methanol-diesel is higher than diesel-gasoline, regarding RON (research octane number, which is usually used to assess the reactivity of fuel. For Methanol it is 106, and for gasoline it is 95.6). Thence, methanol/ diesel fuel is capable of providing more efficient control on ignition timing and burning rate compared with gasoline/diesel in RCCI combustion strategy. Hence, in this study methanol and diesel fuels has been used for RCCI modeling.

Combustion model effects on autoignition and combustion process and also pollutant formation in the combustion chamber for of a DI diesel engine investigated by Arif [2]. The modelled results were validated by comparing predictions against corresponding experimental data for a diesel engine. Case set up per 3 model shown in Table 1.1 and applying appropriate constant of each combustion model including Eddy Break up Model (EBU), Characteristic Timescale Model (CTM) and Extended Coherent Flamelet Model (ECFM) causes the computational result to be in agreement with experimental results.

Table 1.1 : Case set up. [2]

Case	1	2	3
Operating Condition	Diesel	Diesel	Diesel
Combustion Model	EBU	CTM	ECFM
Turbulent Time Scale	0.001	0.001	0.001

Results showed in Figure 1.1 and 1.2 per comparasion of mean pressure, mean temperature, soot and NO mass fraction. In overall, the nearest prediction in comparasion with experimental result is by applying the ECFM model.

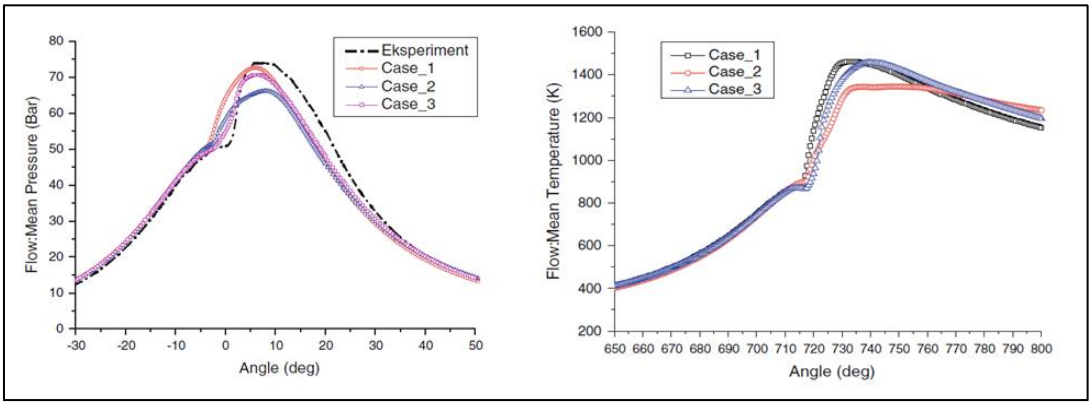


Figure 1.1 : Variation of mean cylinder pressure and temperature with crank angle for all case. [2]

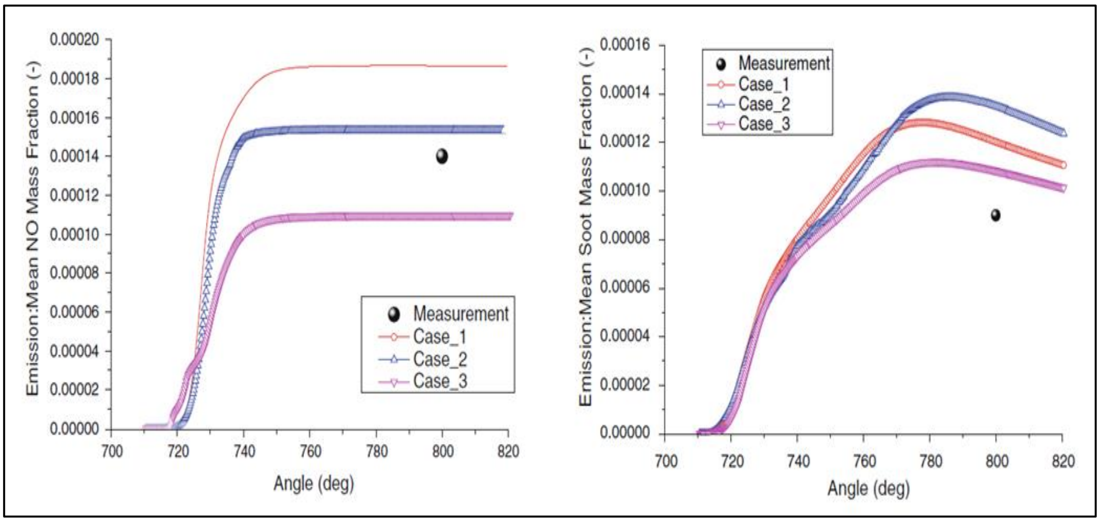


Figure 1.2 : Comparasion of NO and soot prediction for models. [2]

Yaopeng et al. investigated methanol/diesel RCCI combustion engine is studied by introducing two fuel supply systems, i.e. diesel is directly injected into the cylinder and methanol is provided in the intake manifold, the methanol/diesel RCCI combustion is realized [3]. To achieve desirable engine performance, five important parameters including the energy fraction of methanol, initial pressure in cylinder at IVC (intake valve closing), initial temperature in cylinder at IVC, EGR rate, and SOI (start of injection) of diesel fuel were optimized by using NSGA-II in that study. Multiply injection for diesel fuel injection could also affect the combustion and emissions of RCCI engine, which are not considered in the optimization process in order to reduce the complexity.

The results indicated that initial temperature and EGR rate exhibited the most significant effect on engine performance and emissions for their obvious effect on combustion temperature. By varying the local fuel-rich and high-temperature regions, methanol fraction and SOI could dramatically affect NOx (nitrogen oxide) emission. Overall, the RCCI combustion with high methanol fraction and advanced SOI exhibited higher fuel efficiency and lower emissions, as shown in Figure 1.3.

Moreover, it was found that both decreasing EGR rate and increasing initial temperature led to the monotonously increased RI. While decreasing methanol fraction and increasing initial pressure demonstrated the negligible effect on RI at CA50 earlier than 4.3 CA ATDC, which was contributed to their obvious effect on fuel spatial distributions, as shown in Figure 1.4.

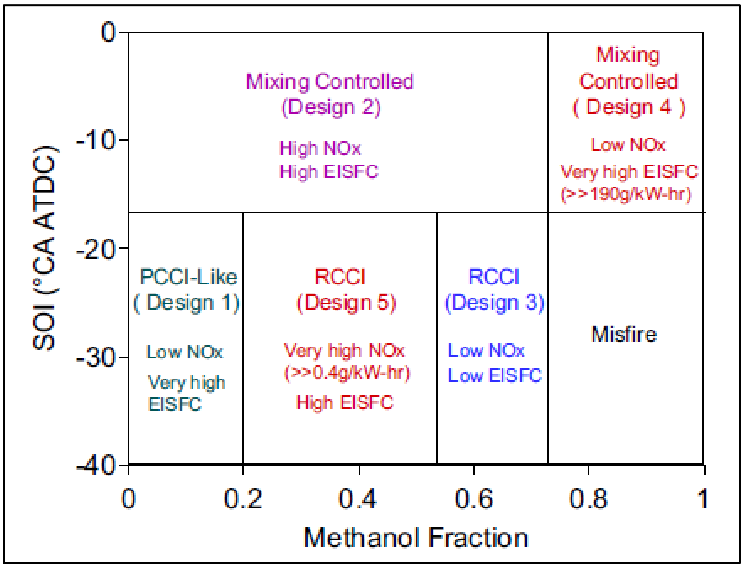


Figure 1.3 : The characteristics of different combustion modes with different SOIs and methanol fractions. [3]

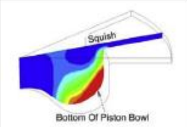
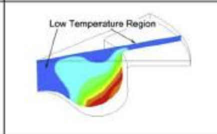
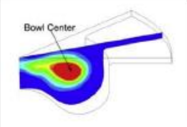
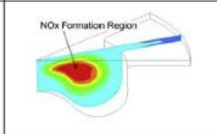
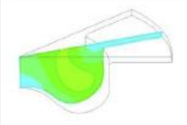
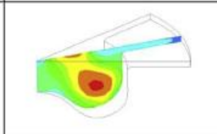
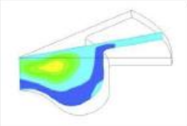
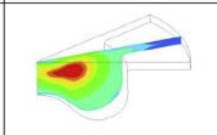
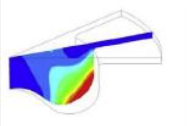
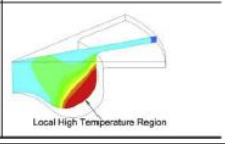
	Operating Parameters	CA50 (°CA ATDC)	Equivalence Ratio	Temperature (K)
(a) Design 1 (PCCI-like)	SOI=29.5 (°CA BTDC) MF=15.96%	-0.52		
(b) Design 2 (Mixing controlled)	SOI=5.8 (°CA BTDC) MF=37.54%	4.12		
(c) Design 3 (RCCI)	SOI=24.4 (°CA BTDC) MF=66.5%	4.35		
(d) Design 4 (Increasing methanol fraction)	SOI=5.8 (°CA BTDC) MF=82.4%	7.66		
(e) Design 5 (Advancing SOI)	SOI=35 (°CA BTDC) MF=37.54%	-4.65		

Figure 1.4 : Different design paremeters with operating conditions. [3]

Regarding that study following conclusions listed:

1. For the optimum solutions, higher initial pressure and a constant level of EGR rate between 27% and 40% should be employed. The optimal initial temperature rises along with the increase of methanol fraction. The RCCI combustion with high energy

fraction of methanol (nearly 70%) and advanced SOI exhibits higher fuel efficiency and lower emissions relatively to other optimum solutions.

2. Initial temperature and EGR rate are the most important operating parameters for the overall engine performance and emissions because of their significant influence on the combustion temperature. Methanol fraction and SOI could dramatically affect NOx and soot emissions by varying the local fuel-rich and high-temperature regions.

3. When the CA50 is earlier than 4.3 CA ATDC, decreasing EGR rate and increasing initial temperature lead to higher RI, while RI shows negligible variation under the acceptable level by decreasing methanol fraction or increasing initial pressure due to their obvious effect on fuel spatial distributions. When the CA50 is later than 4.3 CA ATDC, RI decreases with the retarded CA50 because of the expansion-cooling effect.

4. There is a “sweet spot” of methanol fraction (66.5% in this study) to achieve better fuel efficiency and lower emissions for RCCI combustion. Adjusting the methanol fraction exhibits the most feasible control on ignition timing. The retarded CA50 from the increased methanol fraction contributes to the decrease of RI due to the reactivity-dilution and reactivity-stratification effect of methanol.

Through the investigation in that study, the efficient and stable combustion without the loss of power and fuel economy could be achieved by the methanol/diesel RCCI combustion. The stringent emission regulation could also be satisfied by optimizing the operating parameters. Although the RCCI engine is more complicated with two separate fuel supplement systems, which makes it is a long way to be applied in production engines, the methanol/diesel RCCI engine is still a promising strategy to meet the challenges in the future.

Reitz examined the efficacy of using dual direct injectors for combustion phasing control of high load RCCI combustion[4]. In this study an injection strategy was optimized for a heavyduty compression ignition engine for high load RCCI operation. The fuels used for this study were iso-octane and n-heptane, which are surrogate fuels for gasoline and diesel, respectively. The optimum injection strategy was identified using computational tools—KIVA3V-Release 2, the sparse analytical Jacobian solver, and the multi-objective genetic algorithm NSGA II. The main objective of the work was to examine the effectiveness of utilizing piston geometry for combustion control. After examining the results, the following conclusions were drawn. The 1st injection becomes more effective in combustion control when a large mass was injected close to SOI1:80 deg ATDC. This mass and injection timing combination maximizes the benefit of the evaporative cooling in the squish region. The n-heptane injection mass and timing is the most effective for combustion control. Retarding the SOI by 10 deg crank angle is sufficient to cause misfire. Furthermore, varying combinations of n-heptane mass and SOI produce nearly identical pressure traces and heat release rates. This is because the role of n-heptane injection is to supply the starting energy for the combustion and most of the combustion is carried out by the iso-octane.

1.3 Hypothesis

To overcome diesel engine disadventages, mainly NO and soot emission, RCCI engine targeted with methanol and diesel fuels in separate injection method in number of methanol mass fraction rated mixtures. With this methodology NO and soot reduction expected to be achieved regarding literature research.

2. INTERNAL COMBUSTION ENGINES

2.1 General Definition

An internal combustion engine is an engine where the combustion of a fuel occurs with an oxidizer (usually air) in a combustion chamber and provides power. In an internal combustion engine, power created by force applied to engine components, because of transformation of chemical energy into useful mechanical energy. First commercially successful internal combustion engine was created by Étienne Lenoir, around 1859 and the first modern internal combustion engine was created in 1864 by Siegfried Marcus [5]. Internal combustion engine takes name from the combustion process, which occurs inside of the engine. When combustion occurs outside of engine, it called external combustion engines. For example Steam engines, Stirling engines etc.

In this research, internal combustion engine will be investigated.

2.2 Internal Combustion Engine Classification

Internal combustion engines can be classified regarding stroke number as two and four stroke IC engine. In 2 stroke internal combustion engine, per crankshaft revolution each piston completes a cycle, which consist of 4 process of intake, compression, power and exhaust in 360 deg crank angle. In 4 stroke internal combustion engine, cycle is being completed by movement of piston in 4 process (intake, compression, power and exhaust). Per 2 times crankshaft revolotion cycle completed in 720 deg crank angle.

Cooling is required to remove excessive heat which can cause engine failure, usually from wear, cracking or warping. According to cooling process engines called as air cooled or water cooled. In air cooled IC engines, air is being used as a cooler. Most power tool engines and other small engines are air-cooled. Water cooled engines which use water as a coolant called as water-cooled engines. Most modern automotive engines and larger engines are water-cooled.

According to ignition process IC engines are gasoline, diesel, HCCI, PCCI, RCCI engines.

2.3 Gasoline Engine

Gasoline engines take in a mixture of air as an oxidizer and gasoline and compress it to not more than 12.8 bar. When mixture is compressed, as the piston approaches the cylinder head and maximum stroke, a spark plug ignites the mixture.

Figure 2.1 shows 4 process for 4 stroke gasoline engine P-V change and related crack-piston movement.

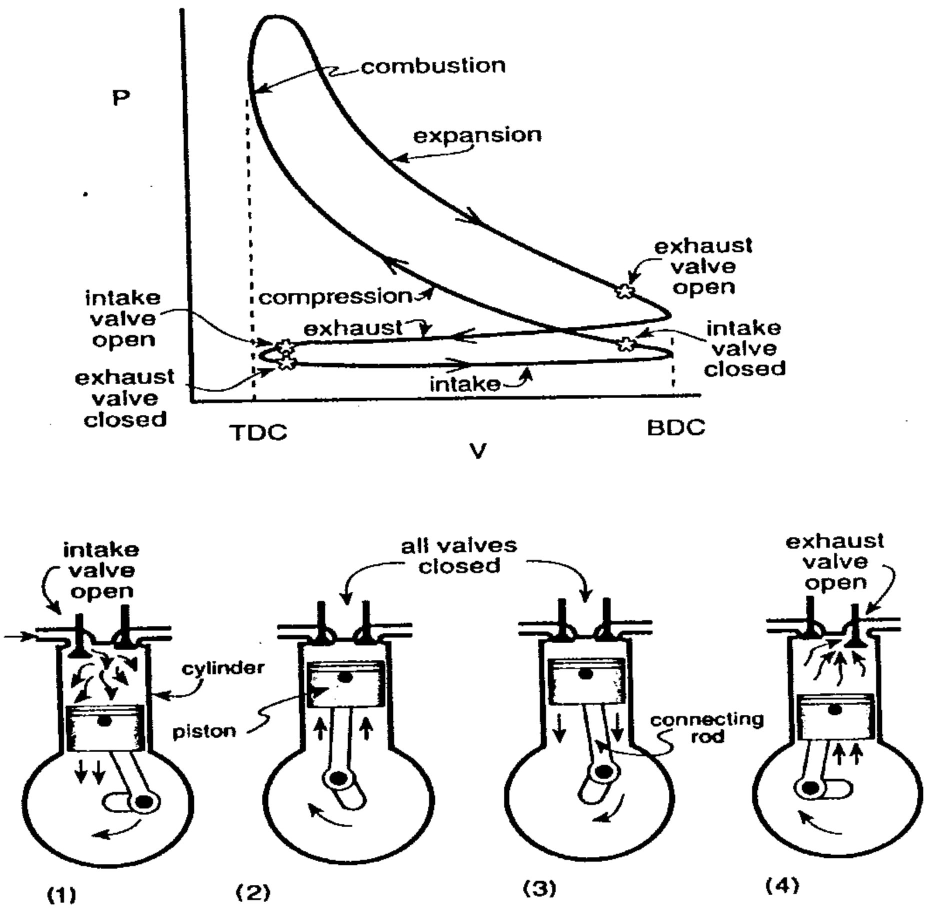


Figure 2.1: Gasoline engine P-V diagram with piston and valve position. [10]

In intake stroke (1), air and fuel mixture taken into combustion chamber. In compression stroke (2), air-fuel mixture taken in intake stroke is compressed from TBC(Top Bottom Center) to TDC(Top Death Center) through piston movement. In power - expansion stroke (3), mixture burns with the help of spark ignition and piston moves from TDC to bottom and power gained. In exhaust stroke (4), Burnt gasses taken out with piston movement from bottom to top.

The theoretical air required to complete combustion of fuel results from the equation of stoichiometry of oxygen/fuel reaction is called stoichiometric air, which means the minimum air in stoichiometric mixture. Figure 2.2 shows emission concerntrations per A/F ratio.

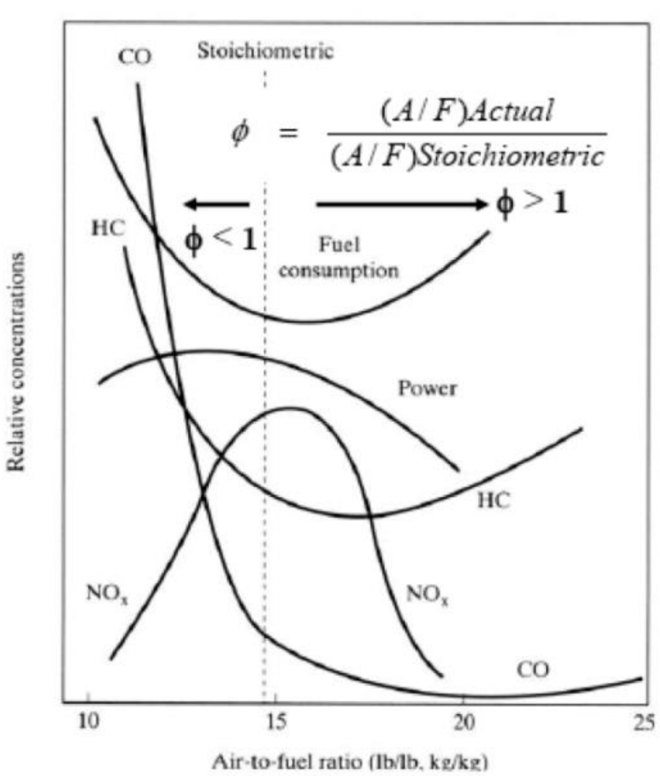


Figure 2.2 : Emission concentrations per A/F ratio. [10]

Regarding following (2.1) chemical reaction of gasoline fuel(C_8H_{18}), CO_2 and H_2O, N_2 gasses occur in the end of combustion and taken out in exhaust stroke, if complete combustion happen.

$$C_xH_y+\left(x+\frac{y}{4}\right)O_2+3.76\left(x+\frac{y}{4}\right)N_2 \rightarrow xCO_2+\left(\frac{y}{2}\right)H_2O+3.76\left(x+\frac{y}{4}\right)N_2 \quad \textbf{(2.1)}$$

If combustion not completed with enough air or fuel, HC, NOx, CO molecules occur, which are harmful for human health in direct/indirect way, as pollutant. To decrease those composites, emission regulations frequently updated that leads automotive producers to achieve those targets to sell cars.

As a result of emission regulations mixture tuning, getting more attention to achieve high combustion efficiency. With an oxygen sensor, unburned oxygen amount in exhaust gasses could be measured and send this valuable information to ECU in order to adjust fuel amount that will get into combustion chamber. Oxygen sensors covered in two type, as lambda and wide band sensors. Lambda sensors act like a switch which says only lean or rich (relative feedback), but wide band oxygen sensors could provide exact λ value (direct feedback) which helps for adjusting mixture more accurate.

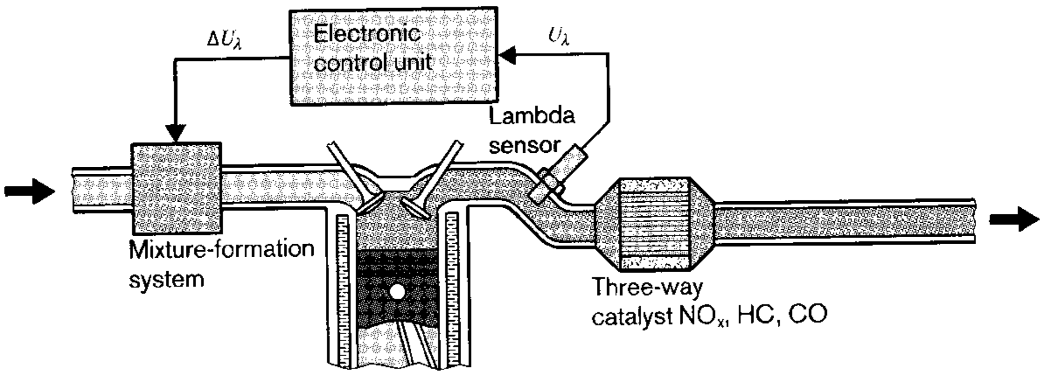


Figure 2.3 : Mixture control system. [10]

λ>1: Lean Mixture (excess air)

λ=1: Stoichiometric Combustion (14.7kg air for 1 kg gasoline)

λ < 1: Rich Mixture (excess fuel)

Regarding output from oxygen sensor HC, CO, NOx amount relation trend shown in below Figure 2.4 per λ(excess air factor) value.

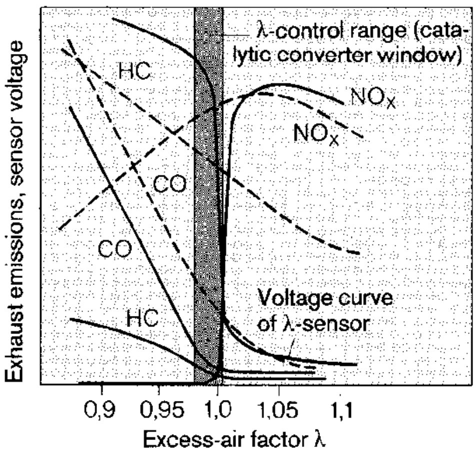


Figure 2.4 : Exhaust emission curves based on λ value. [10]

2.4 Diesel Engine

Diesel engines rely on heat and pressure release created by the engine when its compression process for ignition. Diesel engines take in air only, and shortly before peak compression, spray a small quantity of diesel fuel into the cylinder via a fuel injector that allows the fuel to instantly ignite. Diesel engines dived regarding mixture formation process as pre-combustion chamber injection and direct injection, as shown in Figure 2.5.

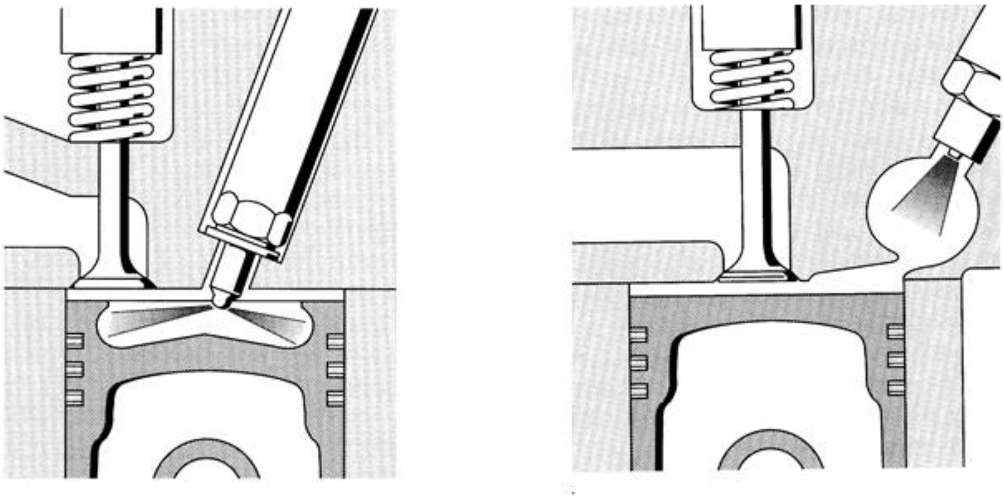


Figure 2.5 : Direct injection(left) and pre-combustion chamber injection(right). [10]

2.4.1 Diesel engine fuel cycle

Combustion stages could be reviewed in four step, as shown in Figure 2.6. After injection of fuel in combustion chamber, there is certain time for delay passed till heat release, which called ignition delay. Premixed combustion phase follows that, which is rapid combustion of the mixed fuel air (with in flammability limits) in a few crank angle degrees. After premixed fuel/air in ignition delay consumed, burning is controlled by the rate when mixture becomes available for burning (fuel vapour-air mixing process). Than late combustion take place and continues in a lower rate well into expansion stroke.

In Figure 2.7 valve timings shown in diesel engine pressure curve based on crank angles. After exhaust valve close(EVC), intake phase starts with increasing pressure and continue till top death center(TDC). With intake valve close(IVC) compression starts. Injection starts earlier than TDC, and combustion starts near TDC.

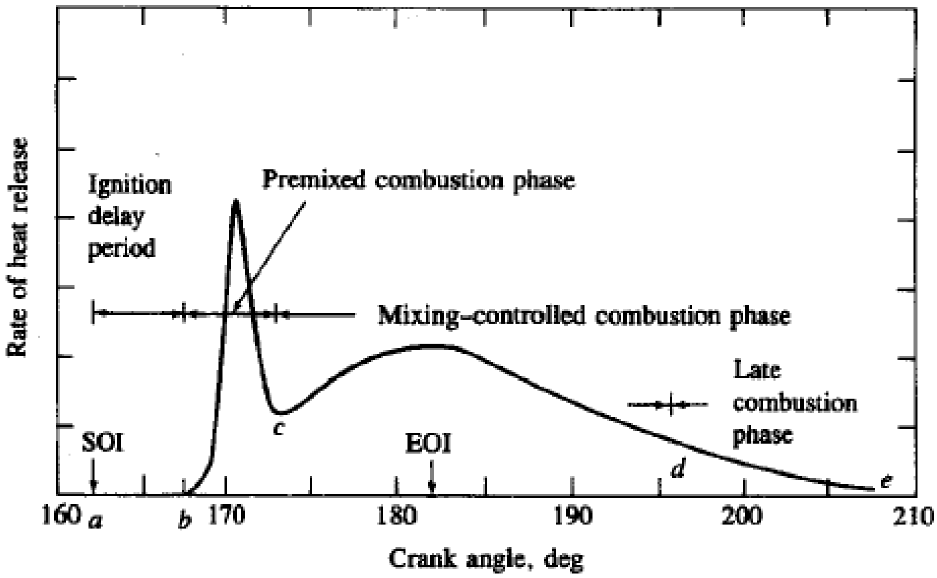


Figure 2.6 : Diesel fuel cycle per crank angle. [10]

Teorically combustion preferred to be started after TDC, in order to not create force against piston ahead when moving through TDC which means negative power. Before reaching bottom death center(BDC), exhaust valve open(EVO) and exhaust process is going on till TDC. Before TDC, intake valve open(IVO) to get air in combustion chamber.

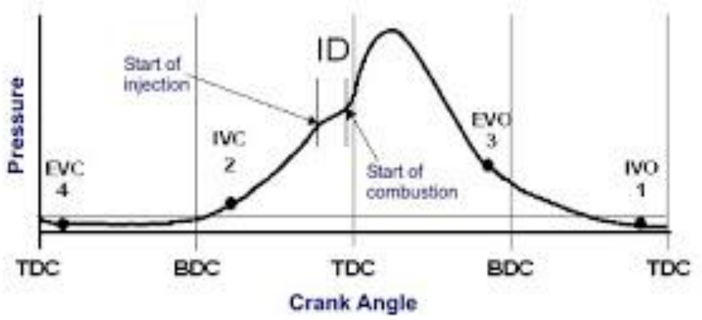


Figure 2.7 : Valve timings per crack angle. [10]

As an example of fuel system, shown below in Figure 2.8. Injection timing is very important to achieve correct mixture to align with regulations. Basically injecton pumps send fuel and it passes through filter and reachs each cyclinder in correct timing defined.

Diesel engine combustion has 4 stroke (intake, compression, expansion, exhaust) as gasoline have.

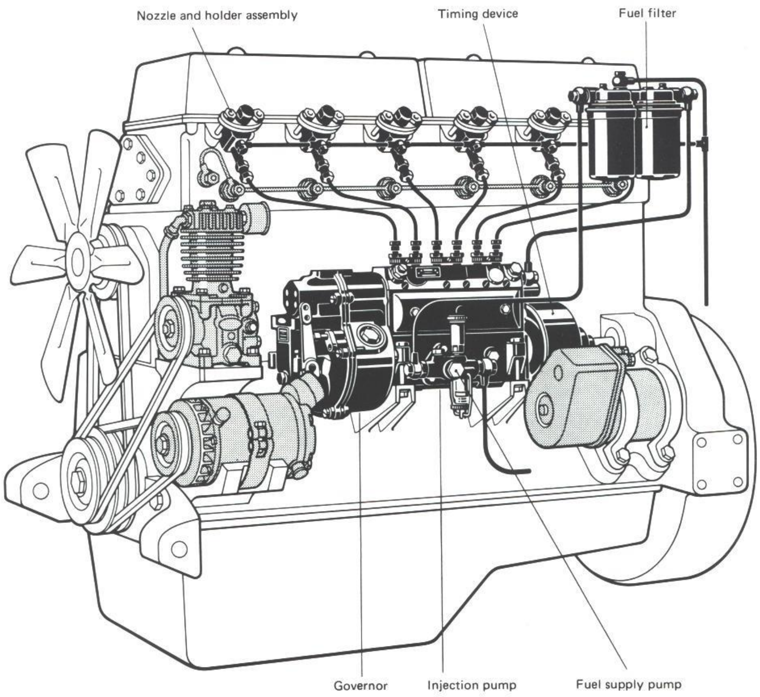


Figure 2.8 : Diesel engine fuel system. [10]

But difference is diesel engine combustion happen automatically without an external device like spark plug, as a result of high squish factor, high pressure and temperature. The other difference is diesel engine takes air in intake process and injects diesel fuel(C13H23) directly into combustion chamber.

Regarding following reaction in **(2.2)**, diesel fuel oxidized and burned.

$$C_xH_y+\left(x+\frac{y}{4}\right)O_2+3.76\left(x+\frac{y}{4}\right)N_2 \rightarrow\ xCO_2+\left(\frac{y}{2}\right)H_2O+3.76\left(x+\frac{y}{4}\right)N_2 \quad \textbf{(2.2)}$$

2.4.2 Diesel engine emission

Diesel engine emissions contain following components: NOx and particulate matters (PM) as diesel inherent products, CO2 and H2O as complete combustion products, CO and HC as incomplete combustion products, O2 and N2 as both reactants and products.

2.4.2.1 NOx emission

Nitrogen oxides (NOx= {N_2O, NO, NO_2}) is a harmful pollutant mostly originating from diesel engines and most critical pollutant. NOx affects both environment and human health, which causes acid rain and ozone smog that mixed with moist air destroying lungs.

NOx formation occurs in following patterns:

- ❖ Fuel NOx, originates from nitrogen bounds from fuel.
- ❖ Prompt NOx, originates from atmospheric nitrogen at the very beginning of combustion process.
- ❖ Thermal NOx, originates from oxidation of atmospheric nitrogen at high temperatures.

2.4.2.2 PM emission

Particulate matter (PM) is defined as any matter in the exhaust of an internal combustion engine that can be trapped on a sampling filter medium at 50°C or less, which originates from the organic and inorganic substances inducted into the engine along with the fuel and air.

One of the major constituents of PM is the carbonaceous matter resulting from the heterogeneous combustion process in diesel engines.

PM source :

- ❖ Both diffusion and premixed flames and in the case of premixed flames by both rich and lean conditions,
- ❖ Dust which is in air and inorganic material which in the fuel or fuel additives,
- ❖ Trace metals from engine component wear,
- ❖ Presence of sulfur in the fuel and lube oil and sulfate particulates which also accumulate humidity,
- ❖ High boiling hydrocarbons and their derivatives, which referred to as the soluble organic fraction (SOF) is composed mainly of lube oil derived hydrocarbons.

2.4.3 Diesel emission control strategies

Diesel emissions reduction can be achieved with following methods:

a. Fuel injection methods:
    - ❖ Higher injection pressure: Increase of pressure creates better pulverization and increase combustion efficiency.
    - ❖ Pre-injection: It eliminates decrease in pressure curve in the beginning of combustion.

❖ Injection rate shaping: Effect combustion efficiency related with propagation of mixture in combustion chamber.
❖ Improved injection timing control

Comon rail system : Common rail system provides high and constant pressure regarding engine demand and cycle. Before common rail system, only 600-700 bars could be achieved with conventionally methods. But, with common rail system, 2500bars even could be achieved. Thanks to high fuel injection pressure, more fuel mass could get inside on fuel with constant pressure, means steady power. Figure 2.9 shows common rail basic schema.

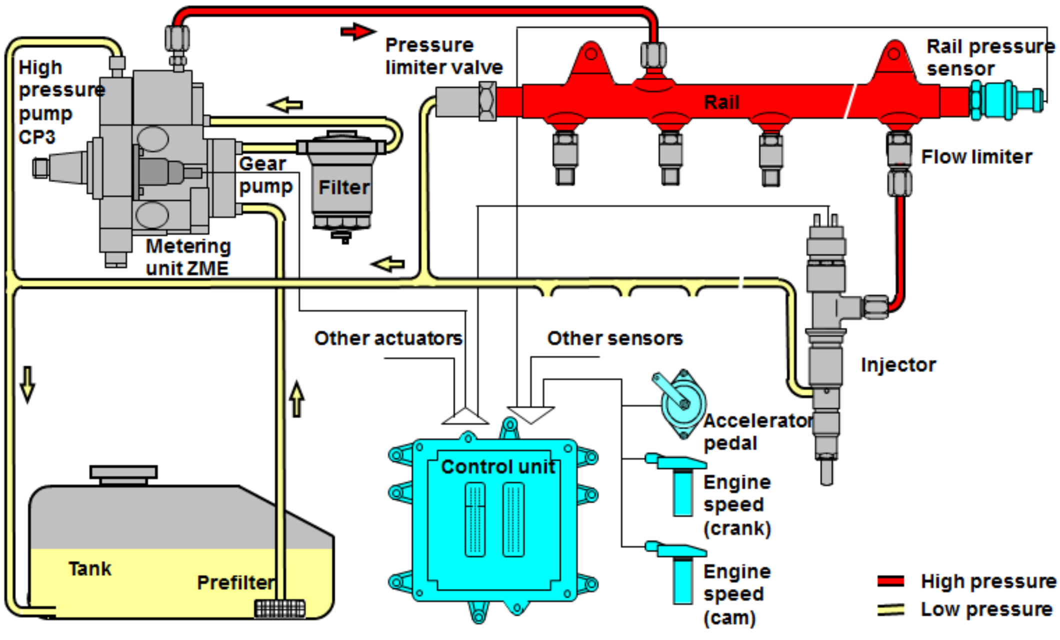


Figure 2.9 : Common- rail system basic scheme. [10]

b. Air systems:

❖ Air pressure, temperature and quantity: This item directly related with how much air get inside of cylinders to oxidize fuel. As much as air mass increased, which gets inside of combustion chamber, as much as fuel can be burned. An example of diesel air system has shown in Figure 2.10.

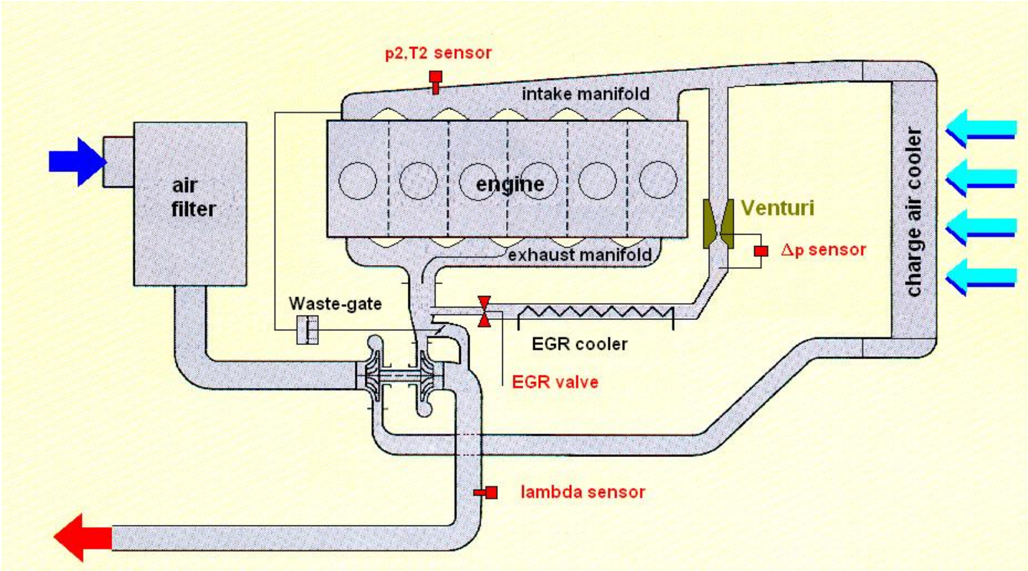


Figure 2.10 : Diesel engine air system. [10]

Exhaust Gas Recirculation (EGR): This sytem directs some of the exhaust gases into intake manifold and use with feed gasses to reduce maximum peak combustion temperatures and reduce NOx formation, as shown in Figure 2.11.

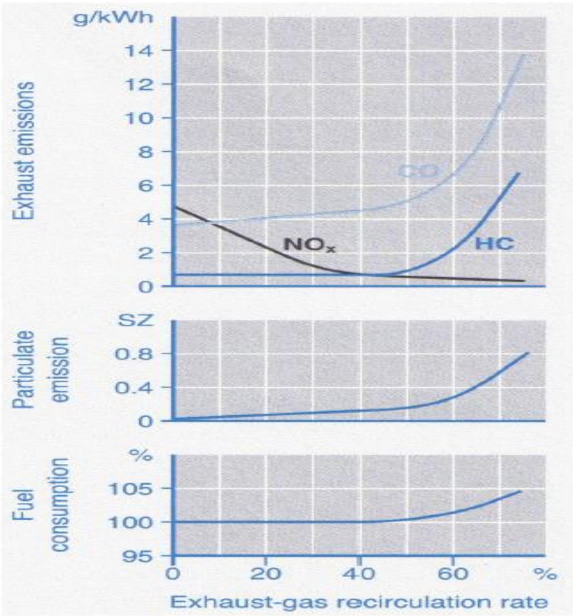


Figure 2.11 : EGR affect on diesel engine emission. [10]

The maing purpose of using an EGR system is to be able to control NOx emissions through;

- ❖ Decrease in rate of combustion and as a result, reduced local peak temperatures due to an increase in inert gas content in the combustion chamber.

- ❖ Reduction in partial oxygen pressure
- ❖ Reduction in exhaust gas mass flow

c. Combustion chamber:

- ❖ Geometry and air motion optimization: It effects airflow movement and is important for creating well mixture of fuel and air.
- ❖ Well-matched with fuel injection system: It is important for fuel injection starting point and pressure to create well-mixed fuel-air in chamber.

d. Aftertreatment Systems: Aftertreatment system components get importance due to tight regulation limits. Aftertreatment components can be further break down as diesel particulate filter (DPF), Lean NOx trap (LNT), selective catalytic reduction (SCR), as shown in Figure 2.12.

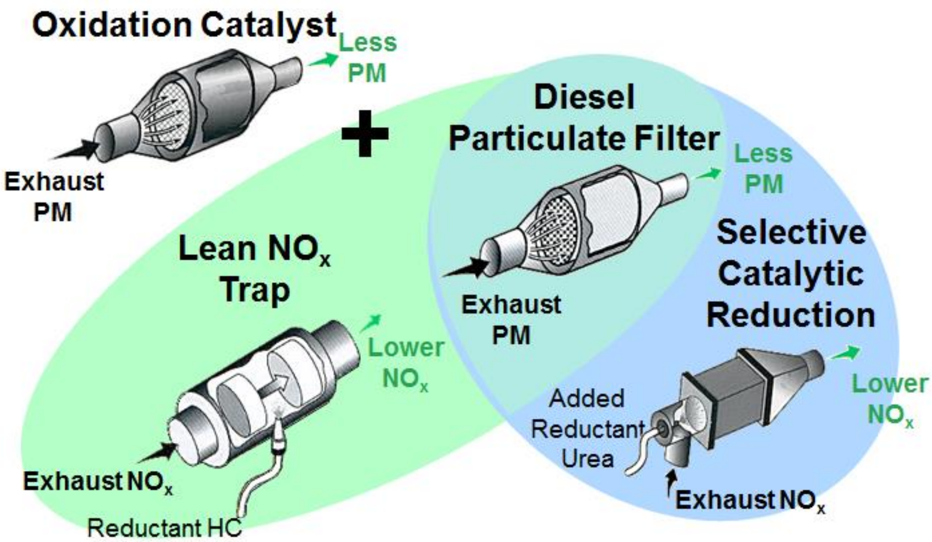


Figure 2.12 : Diesel engine aftertreatment systems. [10]

Diesel Particulate Filter (DPF) It traps carbon particles in the exhaust gasses, and after it is full, it is regenerated. As shown in Figure 2.13, particules couldn't pass DPF cells and go outside and are gathered till limit of capacity regarding emission control strategy. When DPF is fulled with soot particules, regenaration mode runs and burns particules with fuel which comes from post injection period.

Selective Catalytic Reduction (SCR): This catalyst uses ammonia to convert harmful NOx into N_2 and water. Main reactions shown below in Figure 2.14.

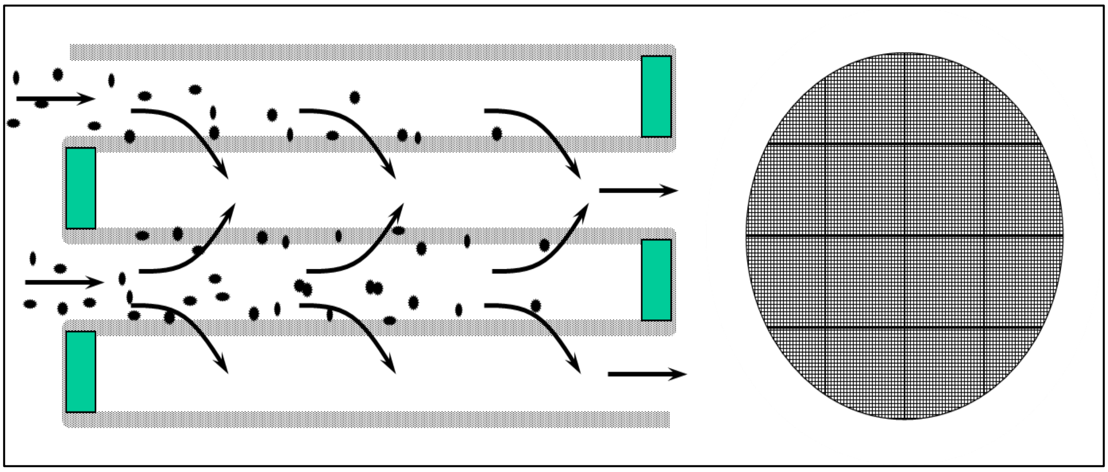


Figure 2.13 : DPF cells working princible. [10]

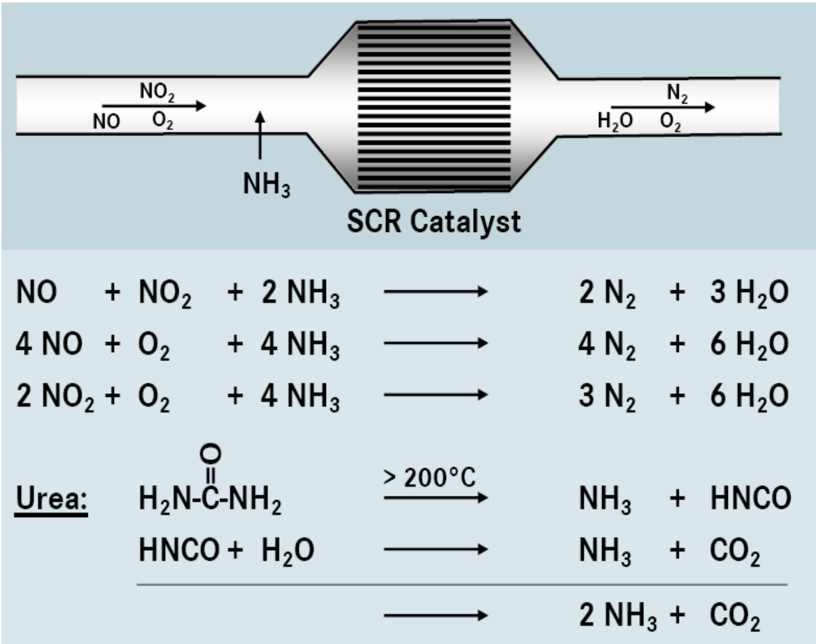


Figure 2.14 : SCR system working principle. [10]

Lean NOx Trap (LNT): During lean engine operation (more O_2 than necessary) catalyst stores NOx and during rich operation (not enough O_2) NOx is reduced to CO_2, H_2O and N_2.

Diesel Oxidation Catalyst (DOC): DO catalysts oxidize any unburnt Hydrocarbons (HC) and Carbon Monoxide (CO) in the exhaust to CO2 and water. Section of DOC shown in Figure 2.15.

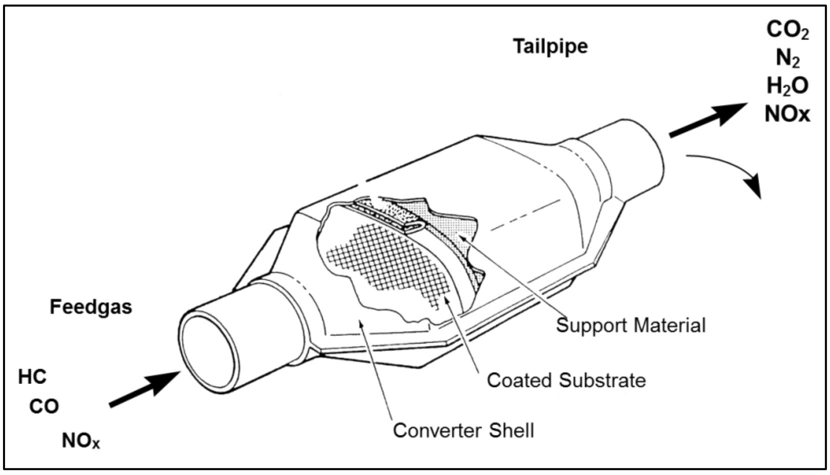


Figure 2.15 : DOC system working princible. [10]

2.5 Premixed Charge Compression Ignition (PCCI) Engine

PCCI engine based on mixture of the fuel with air is provided prior to the initiation of combustion due to early injection of the fuel into the cylinder at low pressure and temperature conditions for autoignition to take place. PCCI engine combustion is controlled by chemical kinetics as mentioned in Sorusbay's notes [6] . With help of applying heavy exhaust gas recirculation rates, cylinder temperature levels can be controlled, in order to dominate ignition process. It helps decreasing Nox and PM emissions in promising levels.

PCCI engine main problems occur at low loads, shown as misfire, and at high loads as rapid pressure rise which leads to uncontrolled ignition timing. Other issues are low thermal efficiency and engine damage.

2.6 Homogeneous Charge Compression Ignition (HCCI) Engine

In HCCI engine lean and homogeneous mixture is compressed until cylinder pressure and cylinder temperature are high enough for autoignition, than combustion starts simultaneously all over the cylinder. Ignition process governed by chemical kinetics and histories of cylinder pressure and temperature, inlet air temperature, compression ratio, residual gas ratio and EGR, wall temperature, as stated in Sorusbay's notes[6].

There are advantages to use HCCI compared to conventional engines. For example, reaction rate is much lower than SI engines due to a higher dilution of the fuel with air or residual EGR gases. High thermal efficiency due to high compression ratio is another advantage, but it comes with rapid heat release rates, which is not preferred.

Low specific fuel consumption with lean mixture and low NOx emissions are achieved by using residual gasses in HCCI engine. In this method, main difficulty comes with controlling ignition and combustion over a wide range of engine operating conditions, shown in Figure 2.16.

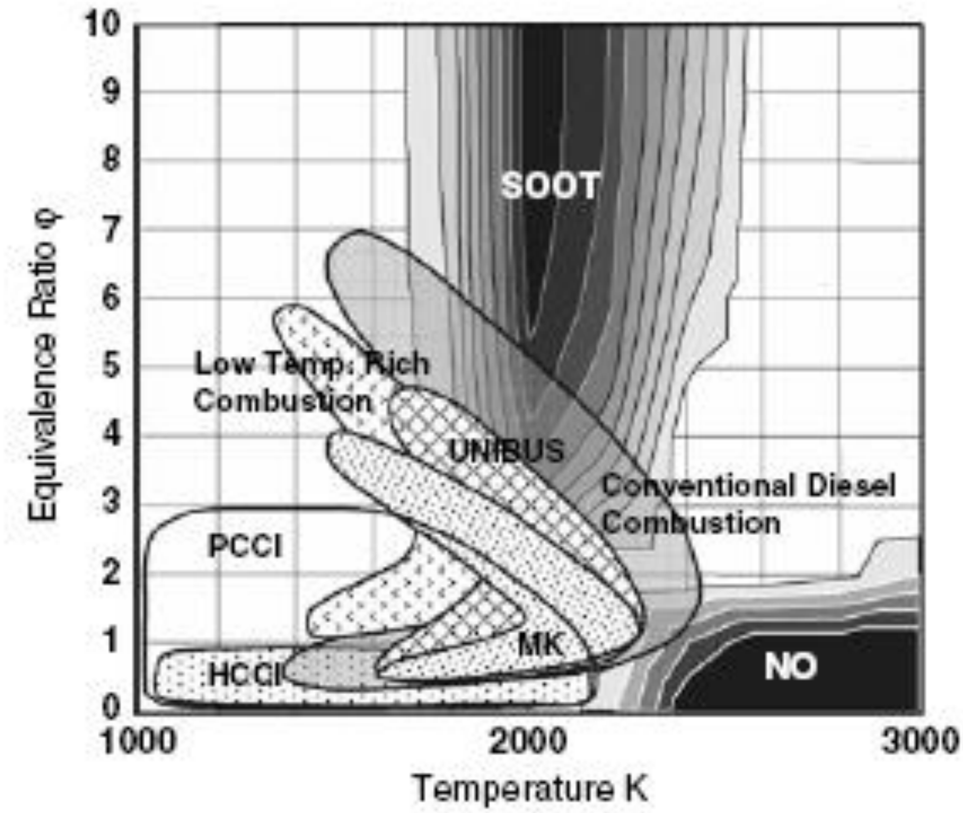


Figure 2.16 : Operating conditions of HCCI and rest of engine types. [10]

2.7 Reactivity Controlled Compression Ignition (RCCI) Engine

RCCI engine mixture is formed with early injection of the fuel into the cylinder. Low octane fuel injected earlier, can be blended with high octane fuel with post injection. In Figure 2.17 Heat release rate per crank angle shown, taken from research [7]. Fuel blend ratio and injection timing are the parameters for control. Varying the mixture ratio of fuel blends with different reactivity levels can provide considerably high thermal efficiencies. Relatively low injection pressures, in comparison to fuel injection systems used in modern diesel engines, provide energy saving. Low temperature combustion reduce NOx emissions while the level of uniformaty of the mixture reduce PM emissions.

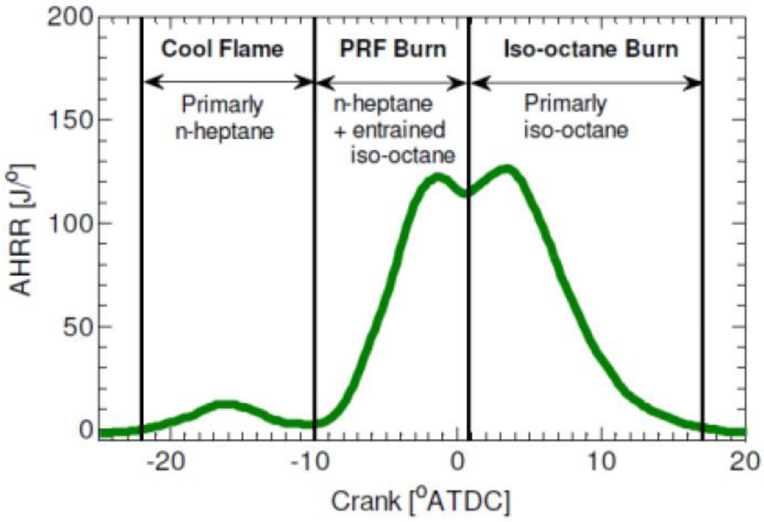


Figure 2.17 : RCCI engine AHRR graph per crank angle. [7]

3. DIESEL ENGINE MODELING

3.1 Reference Engine Attributes and Bowl Dimensions

Cargo Truck Ecotorq 9 liter 380PS Diesel DI engine has been used for experimental test set up in FORD OTOSAN facilities in this study to verify software model results in test labratories. Specifications and operating conditions of the engine are shown in Table 3.1 below.

Table 3.1 : Engine specifications.

Engine Attributes	Descriptions
Model	Ecotorq 9L 380PS DI
Engine Type	Diesel DI
Number of Cylinder	6
Number of Valve per Cylinder	4
Squish Height [m]	0.001
Connecting Rod Length [m]	0.2307
Bore [m]	0.115
Stroke [m]	0.144
Compression Ratio	17.6
Combustion Chamber Shape	Bowl in piston
Injector Operation Pressure [bar]	1850
Injector Hole Amount	8
Injector Hole Diameter [mm]	0.171

Schematic diagram of system is shown in Figure 3.1. In this study, dynometer results gathered from engine, incylinder pressure and temperature and fuel consumption per hour. AVL Fire ESE Diesel program used for mesh and analyze. Results gathered from AVL Fire Workflow Manager Module.

After modeling of the combustion chamber, the initial and boundary conditions should be defined. After creating the moving mesh, the condition of the engine at the end of the induction stroke is considered, as the initial condition.

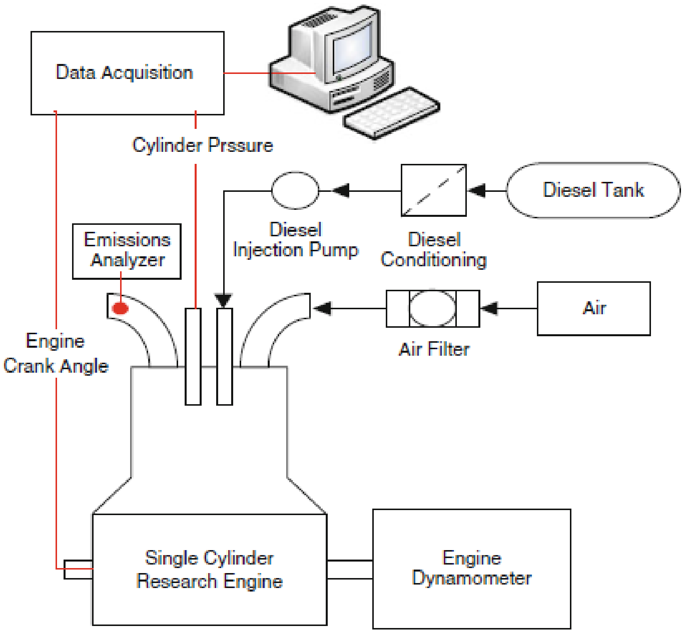


Figure 3.1 : Schematic of experimental setup.

The simulation parameters of the engine are shown in Table 3.2.

Table 3.2 : Diesel engine simulation parameters.

Diesel Engine Operation Conditions	Parameters
Start Angle [Deg]	580 (+40deg ABDC)
End Angle [Deg]	855 (-45deg BBDC)
Cylinder Pressure[Pa]	247229
Cylinder Temperature [K]	384.918
Engine Speed [rpm]	2200
Turbulence Kinetic Energy [m2/s2]	81.96
Fuel Mass Injected per Cycle[mg]	16.57

To calculate turbulence kinetic energy(k) following equation **(3.1)** and **(3.2)** and **(3.3)** has been used taken from research [2]:

$$k = {}^{3}/_{2}\, u'^{2} \qquad \textbf{(3.1)}$$

$$u' = 0.7 * c_m \qquad \textbf{(3.2)}$$

Mean piston velocity(c_m) is defined as follows:

$$c_m = \frac{2*n*S}{60} \qquad \textbf{(3.3)}$$

where, n is the engine speed equals to 2200 rpm and S is the stroke of the engine that equals to 144 mm. Regarding that kinetic energy found as 81.96 m^2/s^2.

3.2 Mesh Size Independence

Piston geometry has been created via sample piston geometry in AVL Fire ESE Diesel. As second step, grid generated as a set of computational meshes covering 360° degree crank angle.

AVL Fire program creates mesh automotically without using additional mesh programs. The 3D mesh of the modeled engine piston bowl is shown in Fig. 3.2.

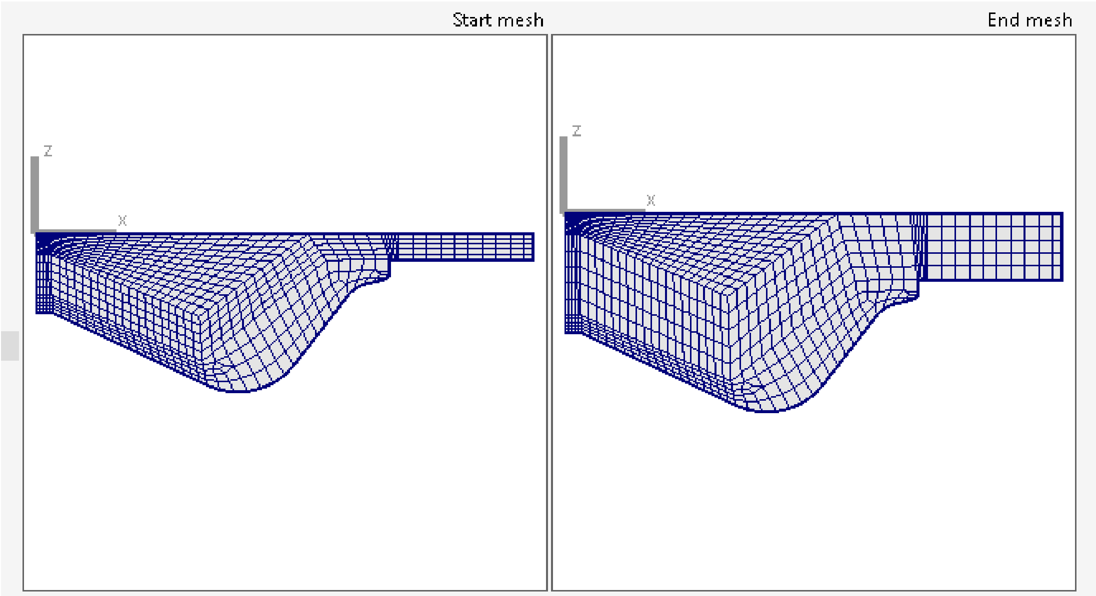


Figure 3.2 : 3D mesh of the modeled engine piston bowl.

As a basic of mesh system, component to be used, needed to be divided into subcomponents to create mesh.

The multi-block structure of grid, containing spray and injector blocks is shown in Figure 3.3 which is pre-process to create mesh correctly. Spray lines and block lines shouldn't be crossed with each other.

In this study 360/8=45° deg sector mesh was used considering that the diesel injector has eight nozzle holes. It helps to decrease simulation times without affecting accuracy of results.

Table 3.3 shows mesh variants have been studied in this work. To achieve mesh independency mesh variants runned from 0.0005 to 0.0030 mean mesh cell size.

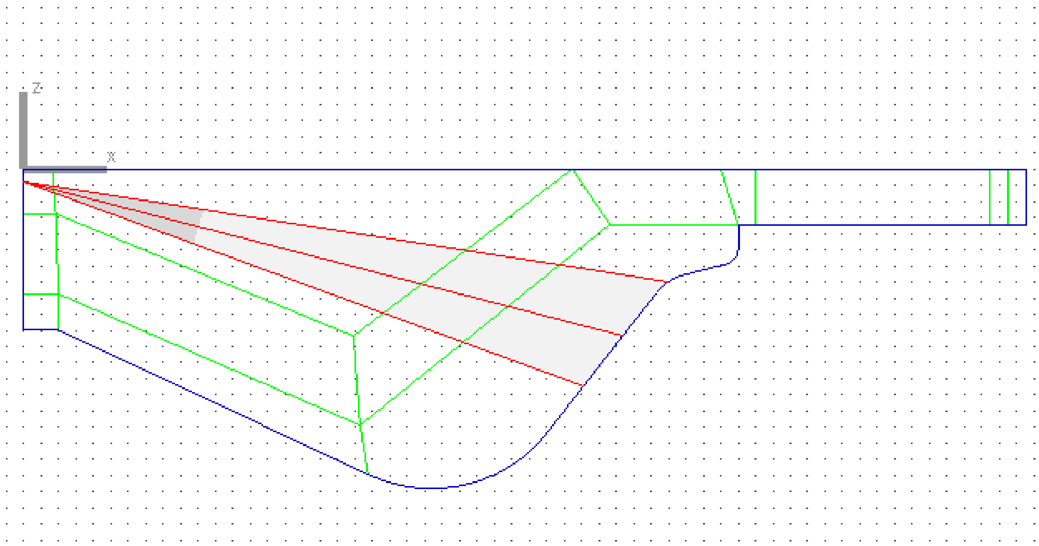


Figure 3.3 : The multi-block structure of grid, containing spray and injector blocks.

Table 3.3 : Various mean mesh size applications.

Mean Mesh Cell Size[m]	Total Number of Mesh Cell	Comments
0.0005	-	No run- mesh size too small
0.0010	47424	Successful
0.0015	32215	Successful
0.0020	-	No run – computation stopped
0.0030	13332	Successful

Regarding mean pressure per mesh variants in Figure 3.4. does not show difference larger than 0.6 bar. Mean temparature values also not show variaty in Figure 3.5. Accumulated heat release values in Figure 3.6 show the similiar proximity between mesh variants.

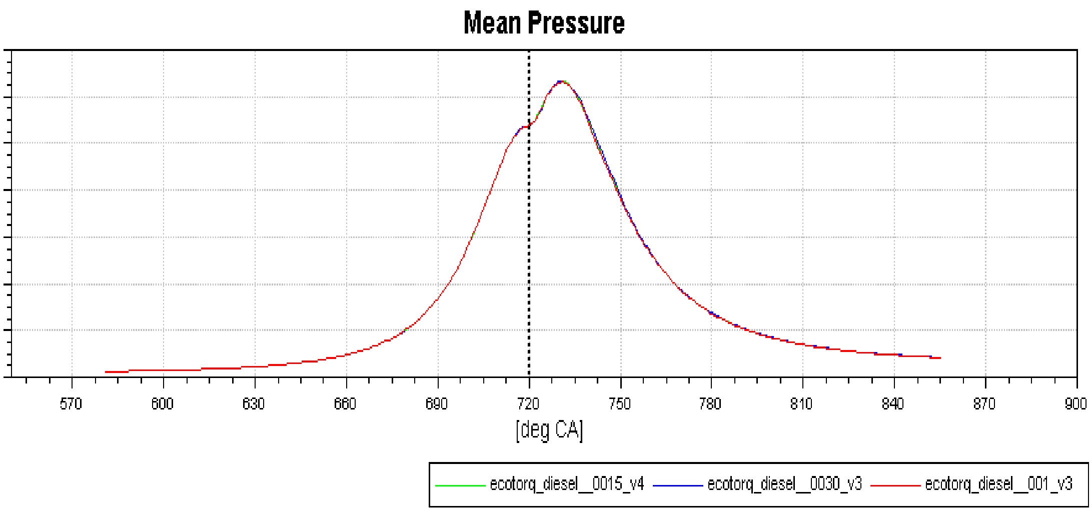


Figure 3.4 : Mean pressure results per mesh size.

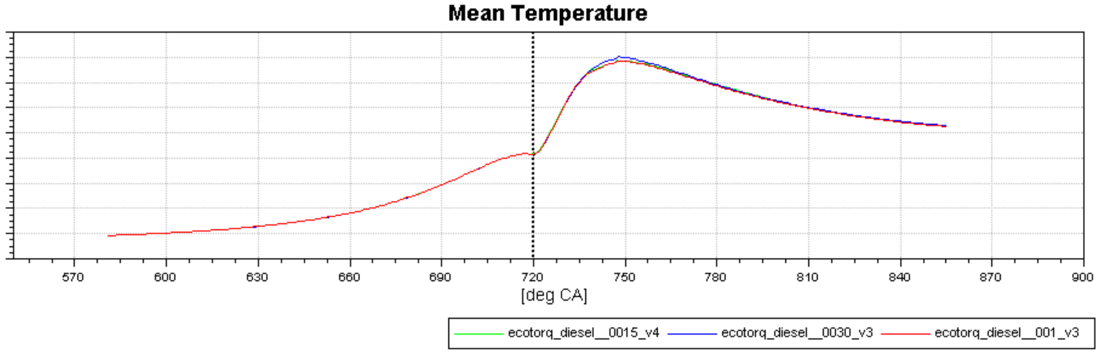


Figure 3.5 : Mean temperature results per mesh size.

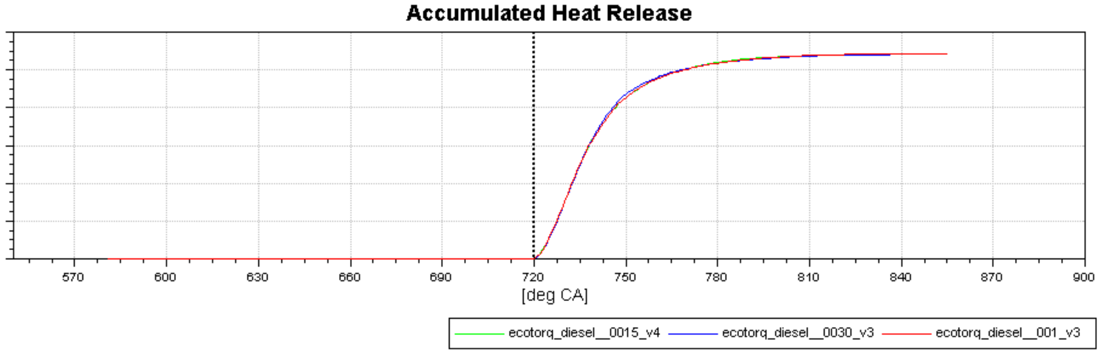


Figure 3.6 : Accumulated heat results per mesh size.

In AVL Fire Program, crank angle per piston placement shown below;

- 540deg CA : BDC
- 720deg CA: TDC
- 900degCA: BDC

Regarding results, mean pressure, mean temperature and accumulated heat release do not show variaty between results of different mesh size. For that reason final decision will be done after emission results view in Chapter 3.6.

3.3 Cold Flow Model

Cold flow model, which has no fuel injected or no combustion happen, has been run to check initial conditions and piston parameters.

Mesh variants shown in Table 3.4. and result shown below in Figure 3.7 with 0.0015m to 0.003m mesh size variants. Dyno pressure values taken from engine dynometer results. Cold flow model and different mesh variants with combustion turned on models run in AVL Fire ESE Diesel program.

Table 3.4 : Cases for combustion and cold flow run.

Cases	Mesh sizes	Case Names
1	-	Dyno_Pressure
2	0.0015	Cold_Flow_Mean_Pressure
3	0.0010	Mean_Pressure_0010
4	0.0015	Mean_Pressure_0015
5	0.0030	Mean_Pressure_0030

Dyno and AVL Fire results(combustion turned on) show enough approximation to take combustion parameters used for further investigation with 0.0015 mesh variant.

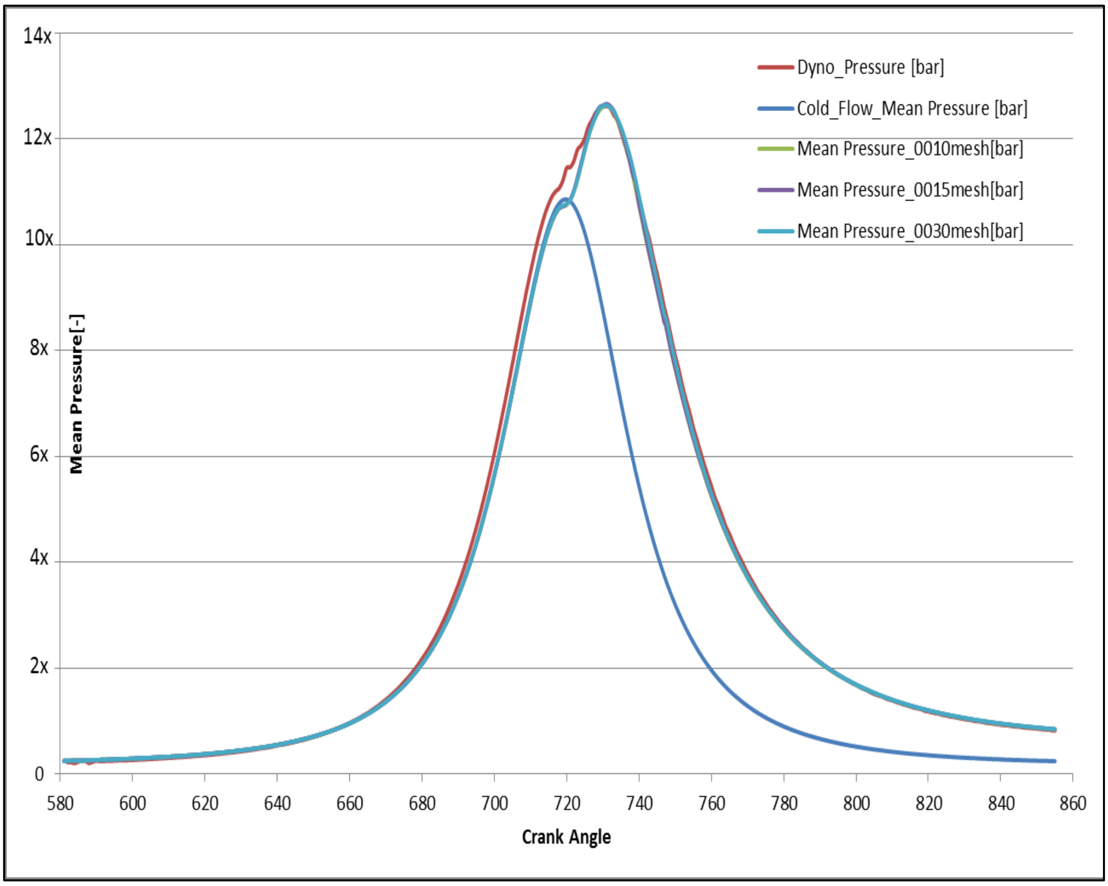


Figure 3.7 : Mean pressure of 5 cases.

3.4 Combustion Model Selection

AVL Fire Program have 7 different combustion models that could be used, explained below as stated in AVL Fire Combustion Module user guideline [9].

3.4.1 Eddy break up model

EBU model is based on the ideas of the Eddy dissipation concept, which assumes that the mean turbulent reaction rate is determined by the intermixing of cold reactants with hot combustion products.

3.4.2 Turbulent flame speed closure model

For the simulation of homogeneously/inhomogeneously premixed combustion processes in SI engines, a turbulent flame speed closure model (TFSCM) is available in FIRE. The kernel of this model is the determination of the reaction rate, can be determined by two different mechanisms via Auto-ignition and Flame propagation scheme , based on an approach depending on parameters of turbulence, i.e. turbulence intensity and turbulent length scale, and of flame structure like the flame thickness and flame speed, respectively.

3.4.3 Probability density function model

Probability Density Function (PDF) approach fully accounts for the simultaneous effects of both finite rate chemistry and turbulence, thus obviating the need for any prior assumptions as to whether one or the other of the two processes determines the mean rate of reaction.

3.4.4 Turbulence controlled combustion model

One of the combustion models available in FIRE is of the turbulent mixing controlled type, as described by Magnussen and Hjertager. This model assumes that in premixed turbulent flames, the reactants (fuel and oxygen) are contained in the same eddies and are separated from eddies containing hot combustion products. The chemical reactions usually have time scales that are very short compared to the characteristics of the turbulent transport processes. Thus, it can be assumed that the rate of combustion is determined by the rate of intermixing on a molecular scale of the eddies containing reactants and those containing hot products, in other words by the rate of dissipation of these eddies.

3.4.5 Characteristic timescale model

In diesel engines a significant part of combustion is thought to be mixing-controlled. Hence, interactions between turbulence and chemical reactions have to be considered. The model described as combining a laminar and a turbulent time scale to an overall reaction rate.

3.4.6 Steady combustion model

The Steady Combustion Model was developed for the purpose of modeling combustion in oil-fired utility furnaces, when one is not particularly interested in the details of combustion, but when the flame dynamics is of crucial importance to the heat transfer in the furnace. It uses empirical knowledge in order to include the influences of evaporation, induction, kinetics and coke combustion in an Arrhenius type expression. The model is well suited for the whole range of typical oil flames, starting from partially pre-mixed to flames governed by several different streams of fuel and air. In order to give physical results for the model, the fuel must be considered pre-mixed with the primary stream of air, since the model already takes the mixing time implicitly into account.

3.4.7 Coherent flame model

The CFM is applicable to both premixed and non-premixed conditions on the basis of a laminar flamelet concept, whose velocity Sl and thickness δl are mean values, integrated along the flame front, only dependent on the pressure, the temperature and the richness in fresh gases. Such a model is attractive since a decoupled treatment of chemistry and turbulence is considered.

Currently, three different CFM’s are available which are described in increasing complexity in below.

3.4.7.1 CFM-2A model

The CFM-2A is applicable for homogeneous and inhomogeneous premixed combustion examples where the determination of the laminar flame speed is only valid within a specific range of the equivalence ratio dependent on the applied fuel.

Outside of this equivalence ratio range the flame speed is zero resulting in no fuel consumption.

3.4.7.2 MCFM model

The MCFM is based on the same concept as the CFM-2A but extensions are available in order to use it for a broader application range. The differences to the standard CFM-2A model are the determination of the laminar flame speed and additional considerations for the flame stretching corrected by the chemical time.

3.4.7.3 ECFM model

The ECFM (E stands for extended) has been mainly developed in order to describe combustion in DI-SI engines. This model is fully coupled to the spray model and enables stratified combustion modeling including EGR effects and NO formation. The model relies on a conditional unburned/burnt description of the thermochemical properties of the gas. The ECFM contains all the features of the CFM and the improvements of the MCFM.

3.4.7.4 ECFM-3Z model

The ECFM-3Z model was developed by the GSM consortium (Groupement Scientifque Moteurs) specifically for Diesel combustion. This is a combustion model based on a flame surface density transport equation and a mixing model that can describe inhomogeneous turbulent premixed and diffusion combustion. The model relies on the ECFM combustion model, previously described. Further it is coupled with an improved burnt gas chemistry description compared to ECFM.

In the past ECFM-3Z combustion model was only applicable for auto-ignition cases, although the code is prepared to handle for both ignition procedures, auto-ignition and spark ignition,. Now the gasoline engine ECFM combustion model can also be activated via the ECFM-3Z mode using all the attractive features such as the general species treatment or separate CO/CO2 oxidation reaction mechanism. So all standard engine applications can be done now with only one identical combustion model.

In this study ECFM-3Z Model has been selected to be used based on capabilities of model for multi component fuel. In this model fuel components used to combined them temporarily to a fuel mixture during the calculation. This means, that effects like auto-ignition and flame propagation shown in Figure 3.8, are handled for this combined fuel within the combustion model. The rate of reaction for each fuel component is finally split up which helps to calculate the consumption of each component separately. The development of the combustion products is based on the consumption of the single components.

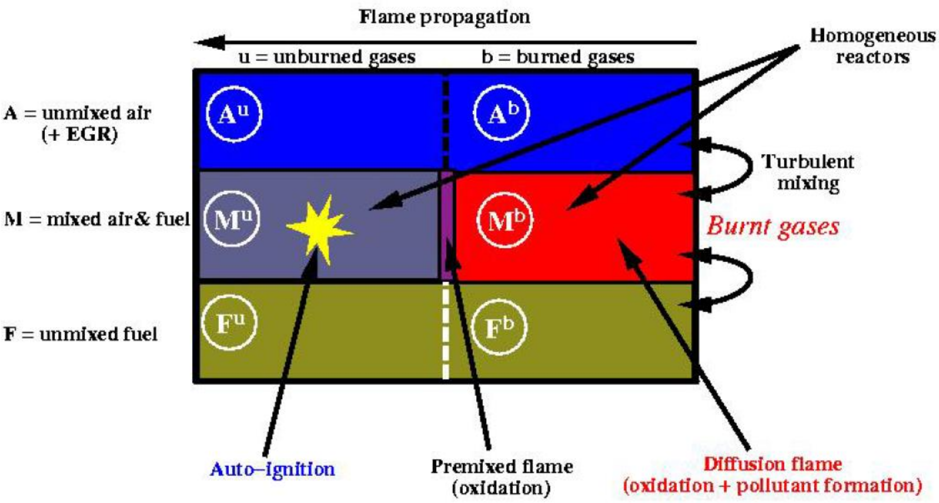


Figure 3.8 : Flame propagation of ECFM-3Z model. [9]

3.5 Combustion Model Parameters

In this study, Coherent Flame Model has been selected both for diesel and RCCI cases due to capabilties mentioned in section 3.4.7.4 under ECFM-3Z Model, shown in Figure 3.9.

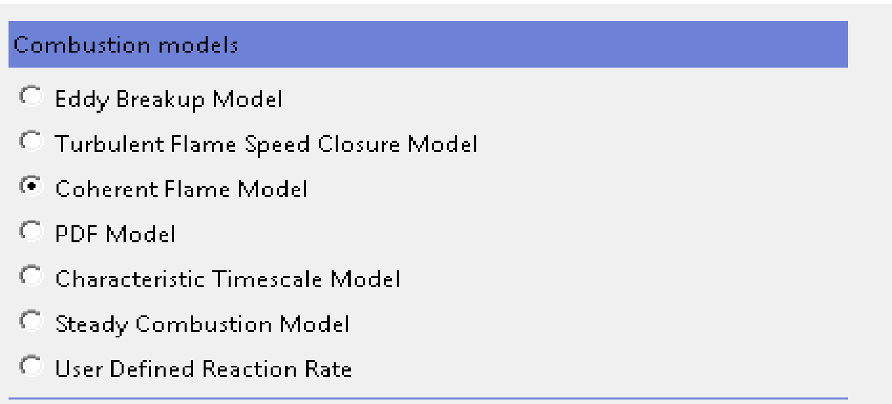


Figure 3.9 : Combustion model that has been selected.

Under Coherent Flame Model, ECFM-3Z has been selected also fo Diesel verification case in order to make sure combustion model make no differense when RCCI model run. In ECFM-3Z Model combustion model parameters has been selected as shown in Figure 3.10. Spark ignition model selected as no. Mixing model parameter influences the transfer of fuel from the pure fuel zone to the mixed zone, selected 1. Auto ignition model represents auto-ignition delay time and Table selected. Autoignition model parameter identify auto-ignition delay time . The inverse of this value is multiplied with the ignition delay time from the databases. This means that values larger than 1 are accelerating the ignition and vice versa. In this study selected as 4. Chemical reaction time value influences the rate of reaction of the fuel during premixed combustion and during auto-ignition, selected as 10000. Extinction temperature is a temperature limit value, when it is below, the fuel is transformed back from burnt status to unburned status, selected 200 degree K.

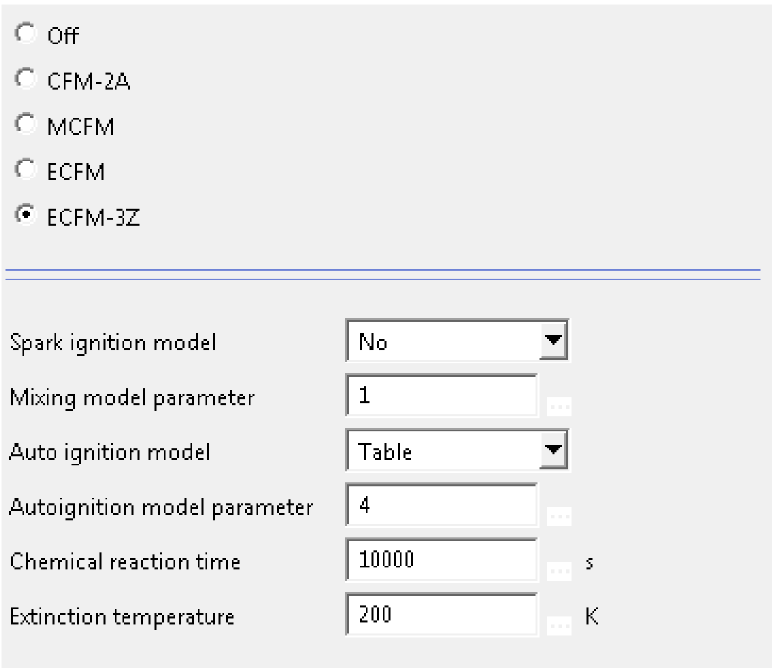


Figure 3.10 : Combustion model parameters.

In the ECFM-3Z model, the transport equations are solved for the averaged quantities of chemical species O2, N2, CO2, CO, H2, H2O, O, H, N, OH and NO. Here, averaged means these quantities are the global quantities for the three mixing zones (that is in the whole cell). Therefore, the term "burnt gases" includes the real burnt gases in the mixed zone (zone bMin Figure 3.9) plus a part of the unmixed fuel (zone bFin Figure 3.9) and air (zone bAin Figure 3.9). This equation is classically modeled as equation **(3.1)**.

$$\frac{\partial\bar{\rho}\tilde{y}_X}{\partial t}+\frac{\partial\bar{\rho}\tilde{u}_i\tilde{y}_X}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{Sc}+\frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{y}_X}{\partial x_i}\right)=\overline{\dot{\omega}}_X \tag{3.1}$$

The amount of mixing is computed with a characteristic time scale based on the k-ε model. During evaporation, it is necessary to specify the amount of fuel going into the mixed zone (from zone F to M=Mu+Mb) and the amount going into the "pure fuel" zone (into zone F=Fu+Fb).

For a diesel spray, the fuel droplets are very close to each other and are located in a region essentially made of fuel. After the evaporation of the fuel, an adequate time is needed for the mixing from the nearly pure fuel region with the ambient air (mixing from zone F and A to M).

In this case, the mixing of fuel with air is modeled by initially placing the fuel into the ‘pure fuel’ zone. So, the fuel which evaporates from a droplet is released in the pure fuel zone F=Fu+Fb).

The main assumption is that the unburned gas composition of air+EGR is the same in the mixed and unmixed areas. Thus if the total amount of oxygen (the oxygen in the mean/total cell) and the unmixed oxygen is known, then the mass ratio of air + EGR mixed over total air + EGR (in the total cell) is known.

For emission equations, following equation **(3.2)** used.

$$\begin{aligned} &N_2 \leftrightarrow 2N \\ &O_2 \leftrightarrow 2O \\ &H_2 \leftrightarrow 2H \\ &2OH \leftrightarrow O_2 + H_2 \\ &2H_2O \leftrightarrow O_2 + 2H_2 \end{aligned} \tag{3.2}$$

3.6 Diesel Model Results and Validation

Mean pressure and mean temperature and accumulated heat release results has been reviewed in Chapter 3.2. In this section mean CO mass fraction in Figure 3.11, soot mass fraction in Figure 3.12 and NO mass fraction in 3.13 will be reviewed for 3 different mesh variants to verify mesh independent diesel model.

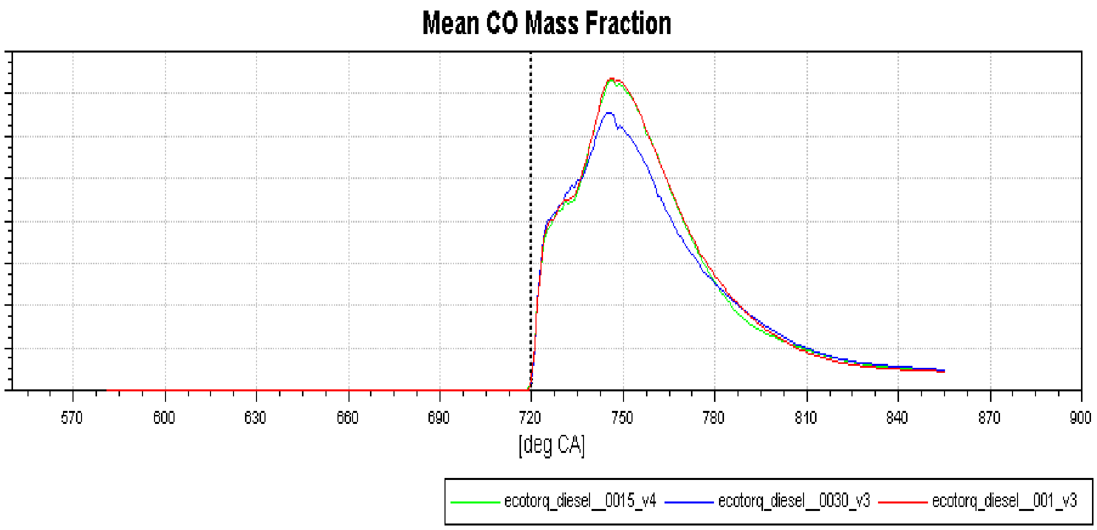


Figure 3.11 : CO mass fraction per mesh variant.

Mean CO mass fraction results shows that 0.001 and 0.0015 mesh cell size variants provide very close results rather than 0.0030 mesh cell size case. That case shows lower CO mass fraction from 740 degree CA to 770 degree CA.

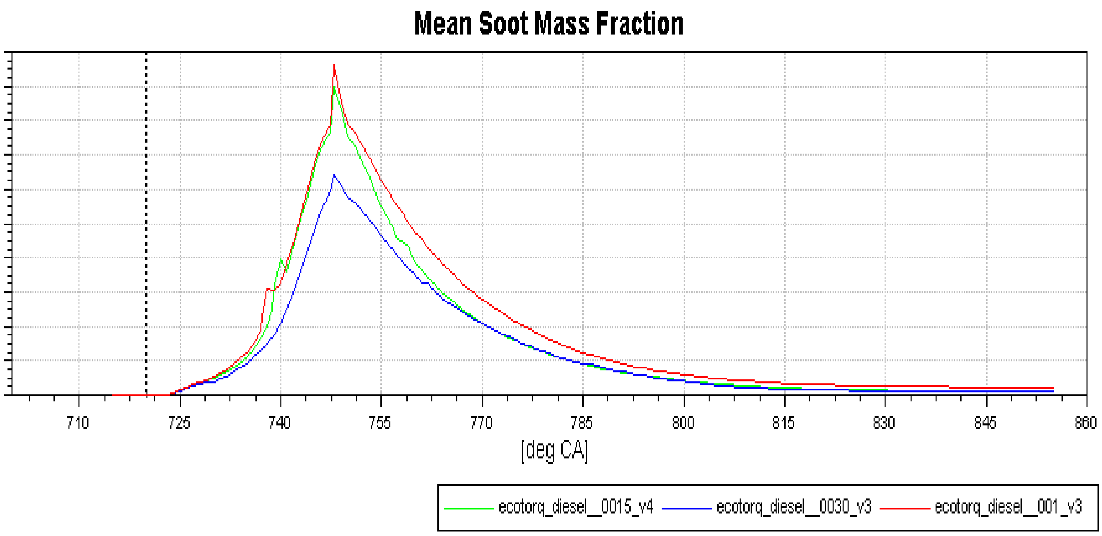


Figure 3.12 : Mean soot mass fraction per mesh variants.

Mean soot mass fraction shows increase on 748deg CA and afterwards soots got burned till exhaust phase. Peak of mass fraction and trend are close to 0.0015 and 0.0010 mesh cases to each other. But 0.0030 shows significant variation for peak mass.

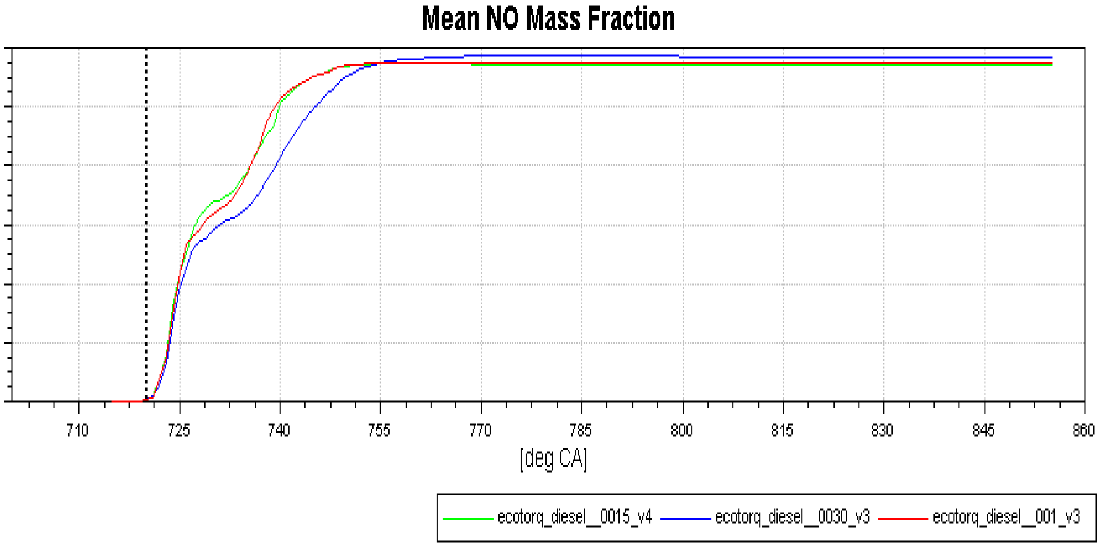


Figure 3.13 : Mean NO mass fraction per mesh variants.

Mean NO mass fraction shows increasing trend till 755degree CA, and afterwards stabilized. 0.0015 mesh size case and 0.0010 mesh size cases have similiar increasing trend, but 0.0030 mesh size case show lower trend rather then first 2 cases. But at 855 degree CA, 3rd case shows higher NO mass fraction from other two.

Regarding foundings in above, 0.0015 mean mesh cell size decided to be used to have enough accuracy without mesh size dependency. In mean pressure, mean temperature and accumulated heat release values are very close to each other. But regarding emission results it shows difference regarding mesh cell size. 0.0015 and 0.0010 results showed close results to each other and with saving simulation time duration, 0.015 mesh size selected in this study to be used.

4. RCCI ENGINE MODELING

4.1 RCCI Engine Model Set up

Regarding diesel engine results 0.0015m avarage mesh cell size selected to apply in RCCI case. ECFM-3Z combustion model selected. All phsical and mesh parameters are same with validated diesel case. Combustion model parameters taken from diesel case with 2 specific change, shown in Figure 4.1. Auto ignition model selected in two-stage. This is the recommended choice, which takes into account databases for different fuel types. Other change has been done, is extinction temperature. Because when multiple injections are calculated, the recommended value is 1500 K or higher.

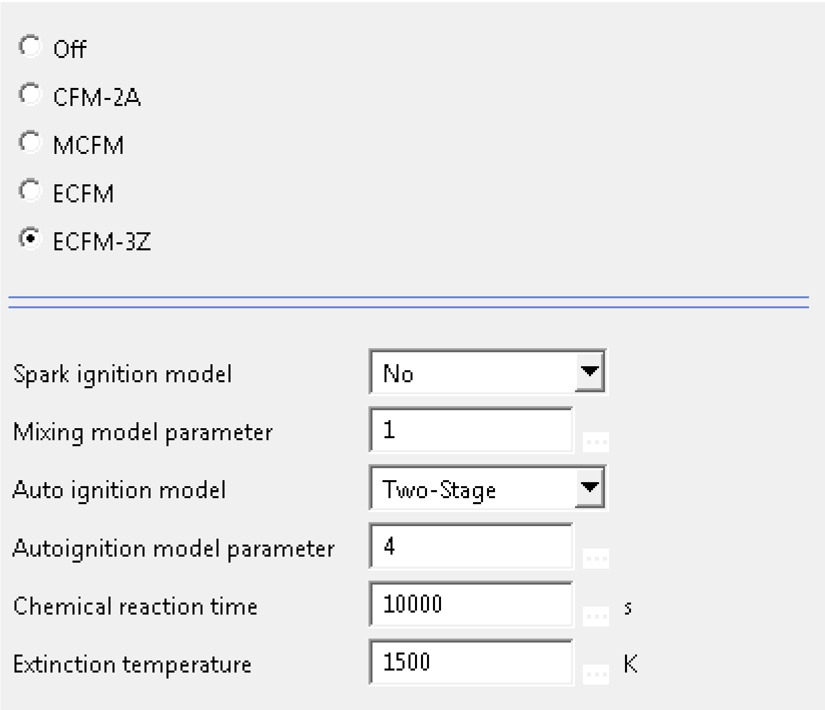


Figure 4.1 : RCCI combustion model and parameters.

4.2 RCCI Cases for Various Diesel-Methanol Mixtures

In this study diesel and methanol selected as fuel for RCCI cases. 8 different methanol mass fraction rated mixtures have been run. In those 8 cases, most promising mixture cases have been run with various SOIs without EGR and with

EGR included way for soot and NO mass fraction decrease opportunity, that will be reviewed in next sections. In total 32 cases has been run.

To define fuel mass for both diesel and methanol, total heat release kept same with the diesel case. Diesel amount has been decreased and related methanol amount calculated regarding following function.

Lower calorific value of diesel (LCV): 42342 J/g

Lower calorific value of methanol (LCV): 19700 J/g

Total heat release: LCV * m

Injection pressure for methanol: 400bar

Injection pressure for diesel: 1850bar

Regarding calculation above, for definite diesel amounts, required methanol injection amounts have been calculated as shown in Table 4.1. Duration of injection is calculated to keep pressure constant for diesel and methanol injections seperately.

Table 4.1 : RCCI engine cases for various mixture mass fractions.

Mixture No	Diesel Amount Inj. [mg]	Methanol Amount Inj. [mg]	Methanol Mass Fraction [-]	Diesel Mass Fraction [-]	Diesel Inj. Duration [CA]	Methanol Inj. Duration [CA]
Case1_main	16.57	0	0	1	30	0
Case2_main	15.00	3.375	0.184	0.816	27.158	6.465
Case3_main	12.00	9.823	0.450	0.550	21.726	18.819
Case4_main	10.00	14.121	0.585	0.415	18.105	27.056
Case5_main	8.00	18.420	0.697	0.303	14.484	35.292
Case6_main	6.00	22.719	0.791	0.209	10.863	43.528
Case7_main	4.00	27.018	0.871	0.129	7.242	51.764
Case8_main	2.00	31.317	0.940	0.060	3.621	60.000

AVL Fire simulations has been run regarding Table 4.1. To get results independent from SOI timings, diesel SOI kept constant in 714.8 CA as base case and methanol SOI kept in 720 CA. Combustion parameters has not been changed. There is 0.03 mass fraction of EGR applied to simulate residual gasses. So those 8 mixture variant cases shows no EGR aplications.

Mean pressure, NO mass fraction and soot mass fraction and total mass results reviewed.

Regarding mean pressure of incylinder results in Figure 4.2, it shows that peak pressure increases, when methanol mass fraction increased till 0.45 without any change in trend till 0.58. With 0.69 methanol mass fraction pressure drops, in case 5. After that break point in case 6 mean pressure trend shows similarity with case 2 and further increase on methanol mass fraction till 0.94, cause decrease on mean pressure peak.

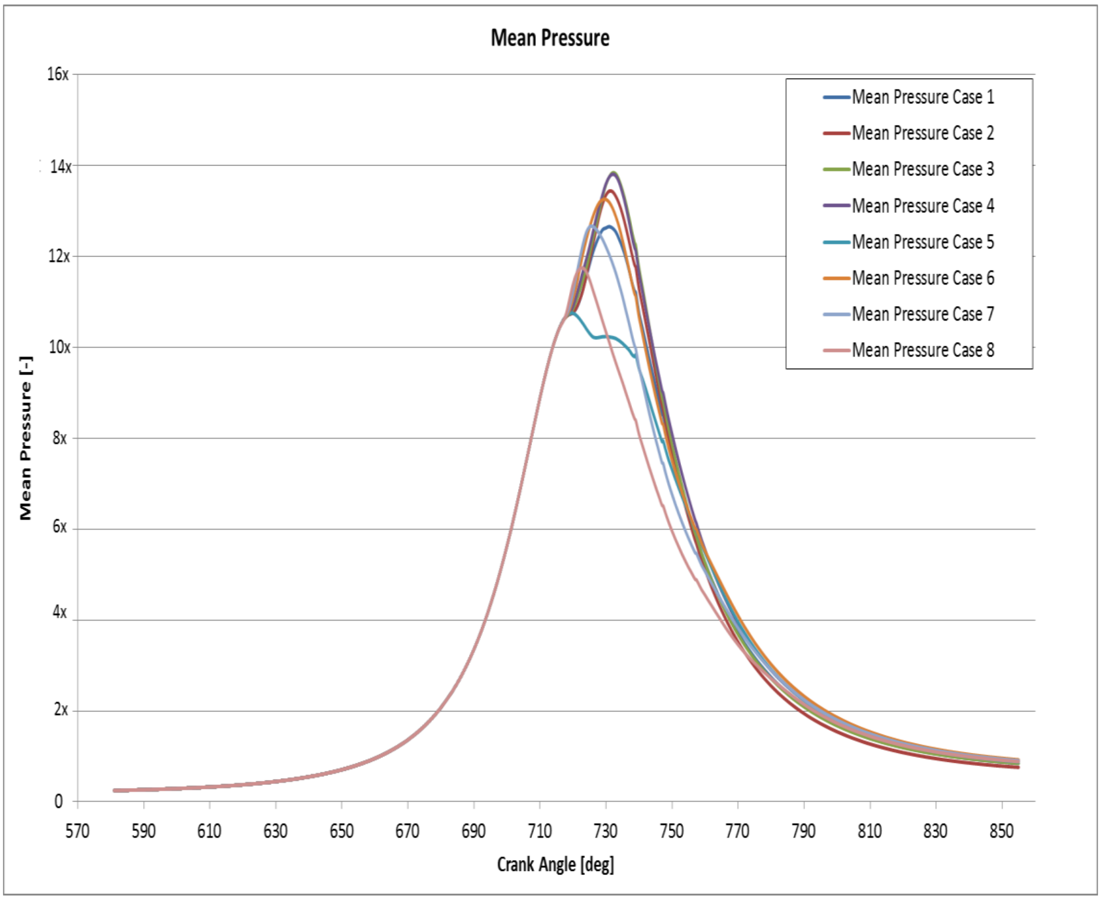


Figure 4.2 : Mean Pressure results of mixture variant cases.

Incresing methanol mass fraction from 0 to 0.585 increase power, than with case 6 decrease on power starts and continue decrease till 0.94 mass fraction of methanol. Case 8 shows lowest NO mass, and also lowest engine power, but NO mass per kW calculated, even %20 decrease on power it shows %96 of NO reduction from base diesel case, as shown in Table 4.2. But it is a result of ineffective burn due to high methanol rate, and can be reviewed also from CO rates in Figure 4.3.

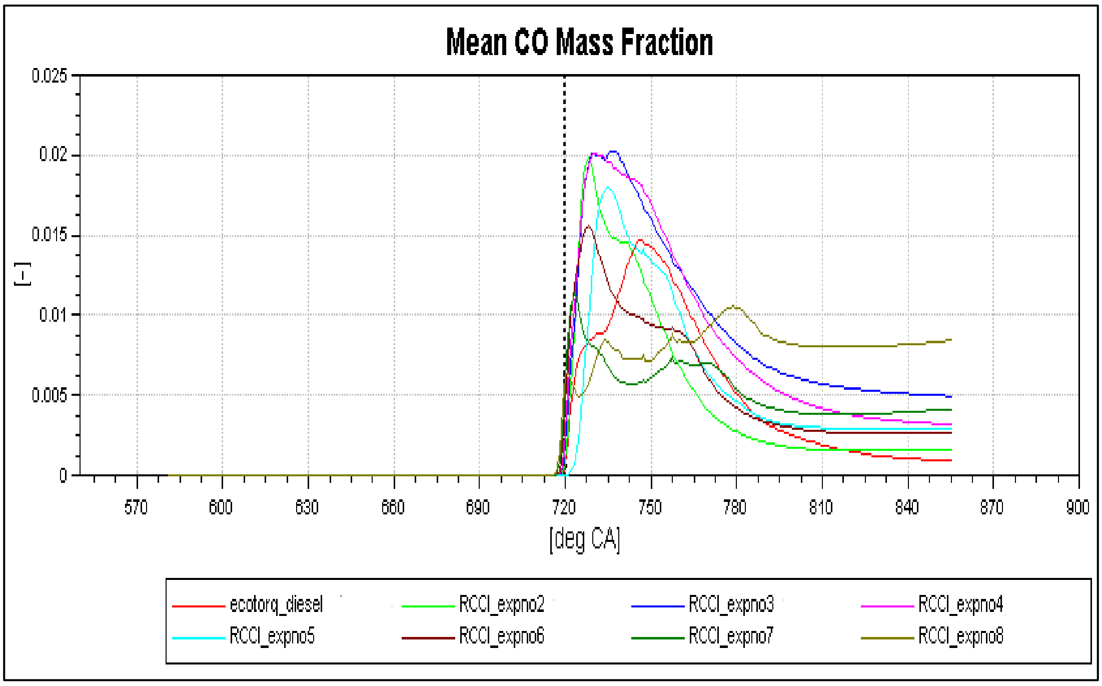


Figure 4.3 : Mean CO Mass Fraction for mixture variant cases.

When case 8 checked for soot ditribution in Figure 4.4, it shows that soot gathered in corner of the cylinder mainly in 855 CA degree.

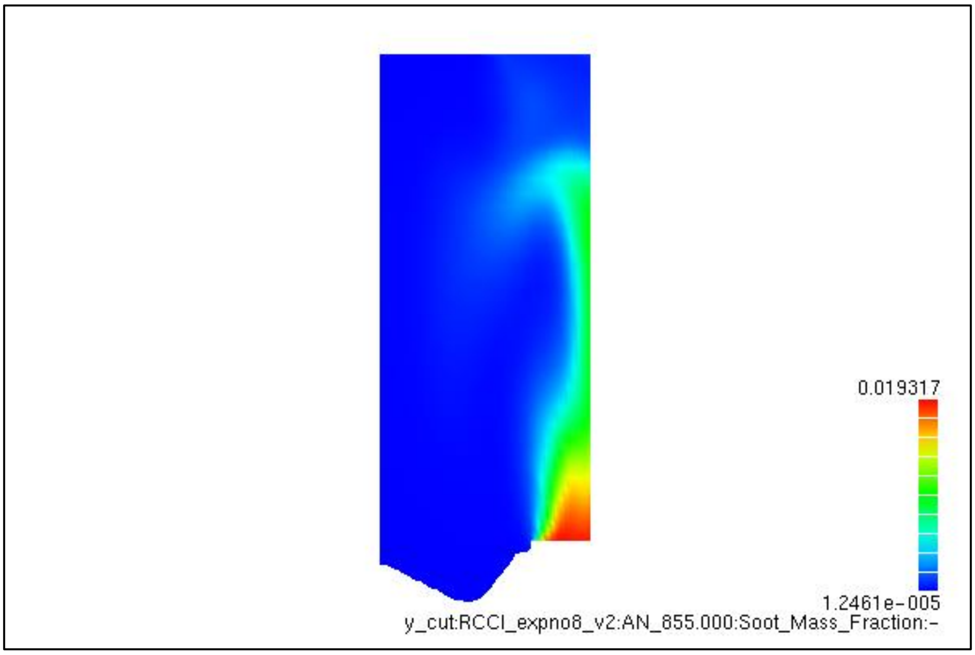


Figure 4.4 : Soot Mass fraction distribution in cyclinder.

Case 5 with 0.69 methanol mass fraction shows %90 NO reduction which follows Case 8, as shown in Figure 4.5. Power decrease on case 5 is only %2 from base case. Furthermore, when checked for CO emission it shows better characteristic rather than case 8.

Table 4.2 : RCCI mixture variant cases.

Mixture No	Methanol Mass Fraction [-]	Power [kW]	NO Mass Fraction [-]	NO [g/kWh]	Soot Mass Fraction [-]	Soot [g/kW]
Case 1_main	0	43.59	2.86E-04	1.43	5.58E-06	0.03
Case 2_main	0.184	41.46	2.28E-04	1.21	2.85E-06	0.02
Case 3_main	0.450	45.11	1.68E-04	0.82	4.33E-04	2.11
Case 4_main	0.585	48.35	1.78E-04	0.81	4.18E-04	1.90
Case 5_main	0.697	42.77	2.70E-05	0.14	5.74E-04	2.96
Case 6_main	0.791	47.62	2.03E-04	0.94	1.08E-03	4.99
Case 7_main	0.871	42.36	1.59E-04	0.83	2.00E-03	10.44
Case 8_main	0.940	35.53	1.03E-05	0.06	2.55E-03	15.87

In all cases NO emissison has been reduced from base diesel case with min %16 reduction from base diesel case.

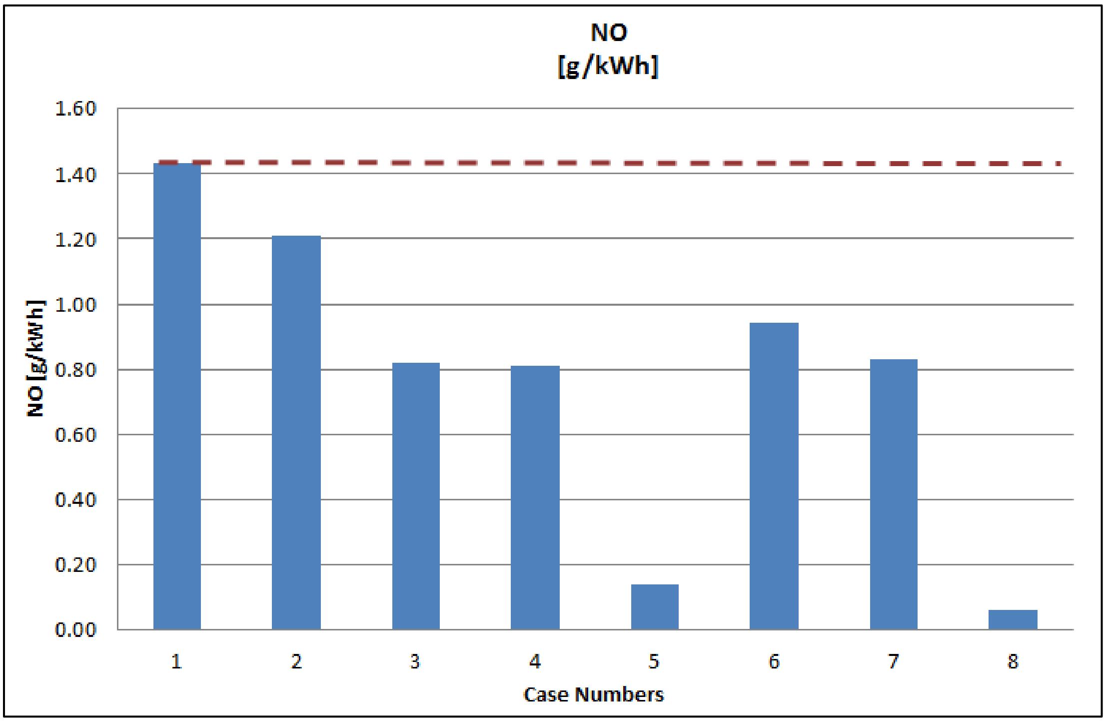


Figure 4.5 : NO emission for mixture variant cases.

When soot amount investigated in Figure 4.6, results shows that case 2 with 0.184 methanol mass fraction is the only case provides soot mass reduction from base diesel case, with %46 reduction of soot per g/ kWh. Case 8 and case 5 which have significant NO reduction over %90 percantage show highest soot mass up to %566 which is another clue of insufficient combustion happen in that case.

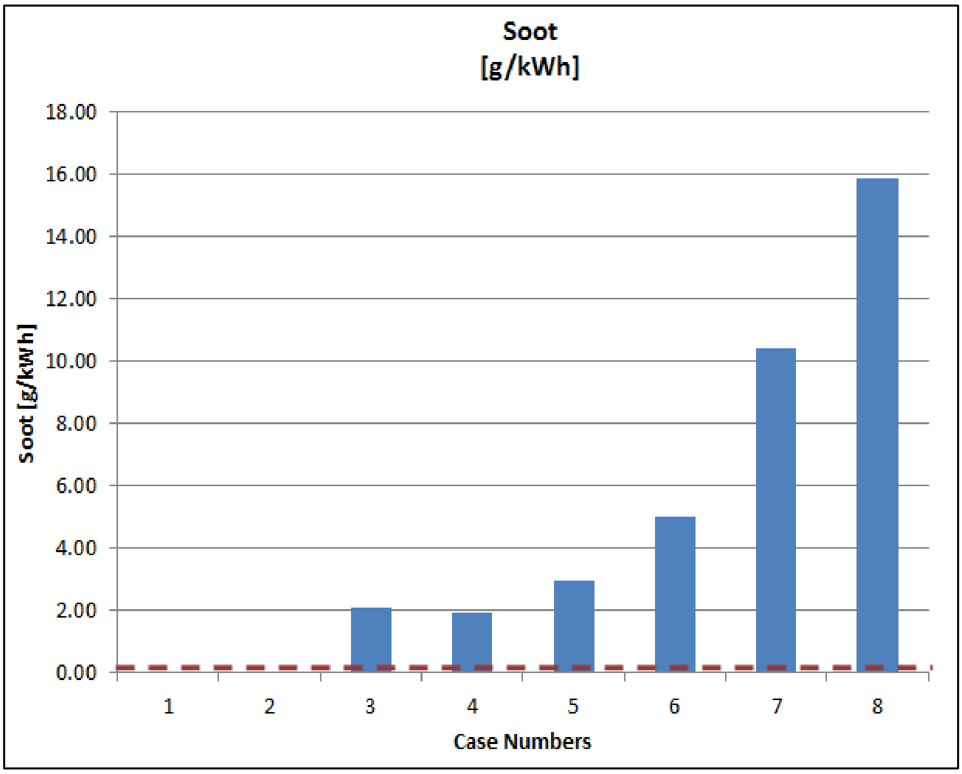


Figure 4.6 : Soot emission results for mixture variant cases.

In overall, when results investigated per mixture variant, NO reduction shown in all cases, but main problematic parameter is soot which shows in all cases very high from base diesel case. Case 2 shows best case when compared with all other cases based on soot and NO emisison, shown in Table 4.3. There is %16 NO reduction and %46 soot reduction achieved with case 2 mixture. Without EGR or advance SOI of methanol and diesel injection, soot mass fraction rates shows significant increase in other cases. Case 2 and 3 and 4 can be investigated with advance SOI and EGR additives to decrease NO and soot to get more improvement on emission basis.

Table 4.3 : Overall NO and soot reduction rates per 8 cases.

Mixture No	NO Reduction [%]	Soot Reduction [%]
case 1_main	-	-
case 2_main	16	46
case 3_main	43	-7451
case 4_main	43	-6717
case 5_main	90	-10484
case 6_main	34	-17765
case 7_main	42	-37244
case 8_main	96	-56677

4.3 RCCI Cases for Various Methanol SOIs for Case 2

Mixture variant RCCI cases and their soot and NO results reviewed previous, in section 4.4. Case 2 provides more promising results for soot %46 reduction and NO %16 reduction in the same time, when there is no EGR and 714.8 CA diesel SOI and 720 CA methanol SOI. In this section, case 2 investigated with various methanol SOI without EGR to find best methanol SOI point to achieve lowest emissions.

In order to achieve correct comparison per cases of case 2, diesel SOI kept as 714.8 CA as same as main case and methanol SOI changed from 715 to 740. Injection durations are constant, for diesel 27.1 CA, for methanol 6.4 CA. Regardingly methanol injection ends shows variaty because of changing SOI, shown in Table 4.4.

Table 4.4 : RCCI cases for various methanol SOIs for case 2.

Case No	Diesel Amount [mg]	Meth. Amount [mg]	Diesel SOI [CA]	Diesel Inj Dur. [CA]	Diesel Inj. End [CA]	Meth. SOI [CA]	Meth. Dur. [CA]	Meth. Inj. End [CA]
2.a	15.00	3.375	714.8	27.1	741.9	715	6.4	721.4
2.b	15.00	3.375	714.8	27.1	741.9	718	6.4	724.4
2.c	15.00	3.375	714.8	27.1	741.9	720	6.4	726.4
2.d	15.00	3.375	714.8	27.1	741.9	725	6.4	731.4
2.e	15.00	3.375	714.8	27.1	741.9	730	6.4	736.4
2.f	15.00	3.375	714.8	27.1	741.9	735	6.4	741.4
2.g	15.00	3.375	714.8	27.1	741.9	740	6.4	746.4

Regarding case set up above and Table 4.4, NO and soot emission investigated. Base diesel case results has been compared, marked with red dot line in Figure 4.7. Lowest NO emission observed in 730 deg CA methanol SOI with %38 NO reduction. Even in highest NO emission observed case, 718 deg CA SOI, NO emission shows %10 reduction from base diesel case .

In soot point of view, increasing SOI after 720 deg CA, all results show higher soot emission from base case marked with red dashed line. Lowest soot emission observed at 718 deg CA SOI, which shows %54 decrease, as shown in Figure 4.8.

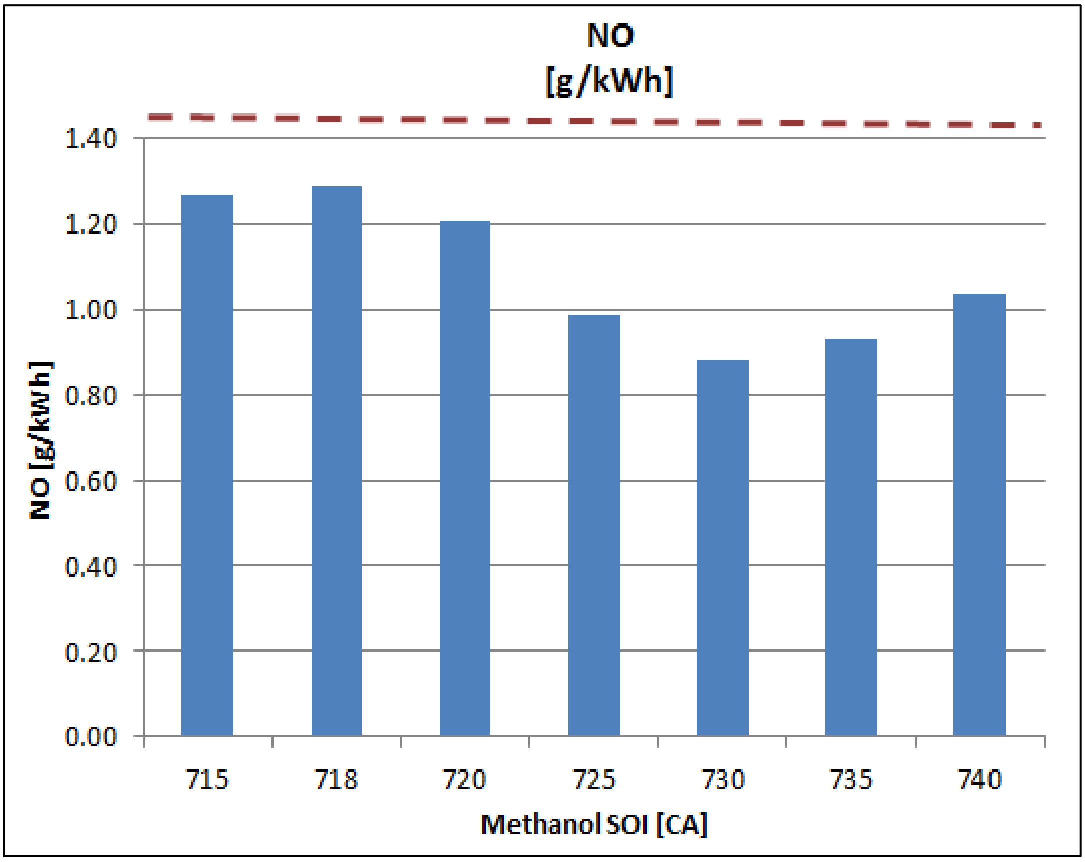


Figure 4.7 : NO emission results for case 2.

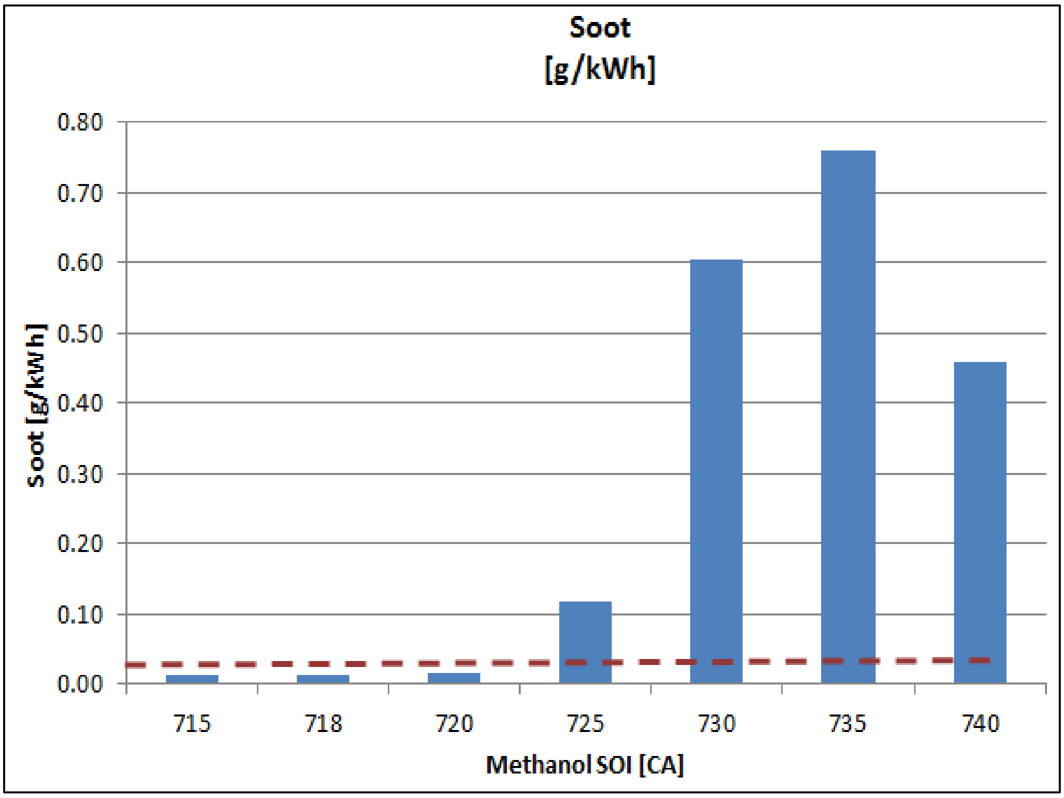


Figure 4.8 : Soot emission results for case 2.

Table 4.5 : Case 2 NO and soot emission reduction rates per SOI variants.

Case NO	NO Reduction [%]	Soot Reduction [%]
2.a	12	53
2.b	10	54
2.c	16	46
2.d	31	-319
2.e	38	-2067
2.f	35	-2616
2.g	28	-1539

Case 2 results show that with keeping mixture amount and diesel injection parameters constant and only changing methanol SOI, NO and soot emiossion could be reduced, shown in Table 4.5. To decrease soot, methanol SOI should be applied before TDC, but this also increase NO mass due to reaching high pressure and temperature gradients as a result of providing enough time to methanol fuel fully mixed with air in combustion chamber and ignate earlier when temperature is much more higher. At 718 deg CA, results show more balance for soot and NO emission to gather both reduction benefit. In that case, even NO emission is higher than other methanol SOI variants, there is %10 NO reduction benefit from base case.

4.4 RCCI Cases for Various Methanol SOIs for Case 3

In this section case 3 will be deeply investigated to get an opportunity to decrease NO and soot without decrease on power for no EGR application. Diesel SOI kept same and methanol SOI timings shows variaty without changing duration of injection period to not affect injection pressure. Methanol mass fraction kept same as 0.45 for all cases and only SOI timing of methanol has been changed, as shown in Table 4.6.

Table 4.6 : RCCI cases for various methanol SOIs for case 3.

Case No	Diesel Amount [mg]	Methanol Amount [mg]	Diesel SOI [CA]	Diesel Inj. Dur. [CA]	Methanol SOI [CA]	Methanol Dur. [CA]	Methanol Inj. End [CA]
3.a	12.000	9.823	714.8	21.7	715	18.8	733.8
3.b	12.000	9.823	714.8	21.7	718	18.8	736.8
3.c	12.000	9.823	714.8	21.7	720	18.8	738.8
3.d	12.000	9.823	714.8	21.7	725	18.8	743.8
3.e	12.000	9.823	714.8	21.7	730	18.8	748.8
3.f	12.000	9.823	714.8	21.7	735	18.8	753.8
3.g	12.000	9.823	714.8	21.7	740	18.8	758.8

NO results shows that, 715 deg CA SOI case provide %49 NO reduction from base case marked with red dashed line in Figure 4.9. As far as methanol SOI time getting later, NO emision increases and right after 735 CA SOI case, NO emission passing base case limit. Figure 4.10 shows soot emission per methanol SOI change.

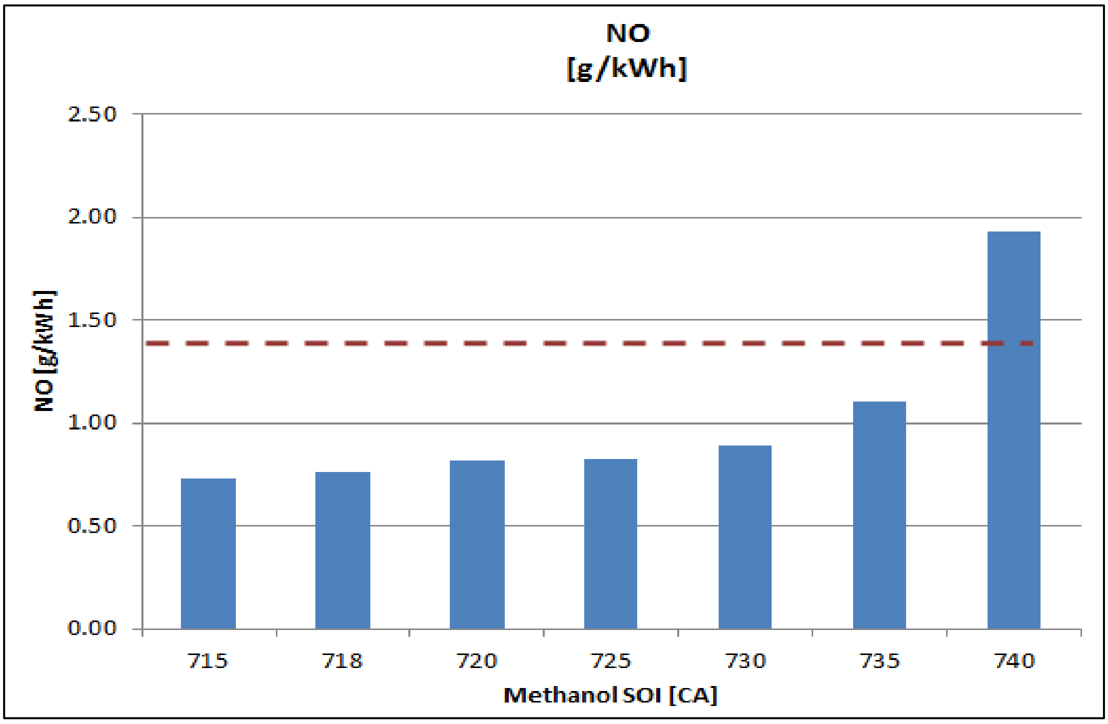


Figure 4.9 : NO emission results for case 3.

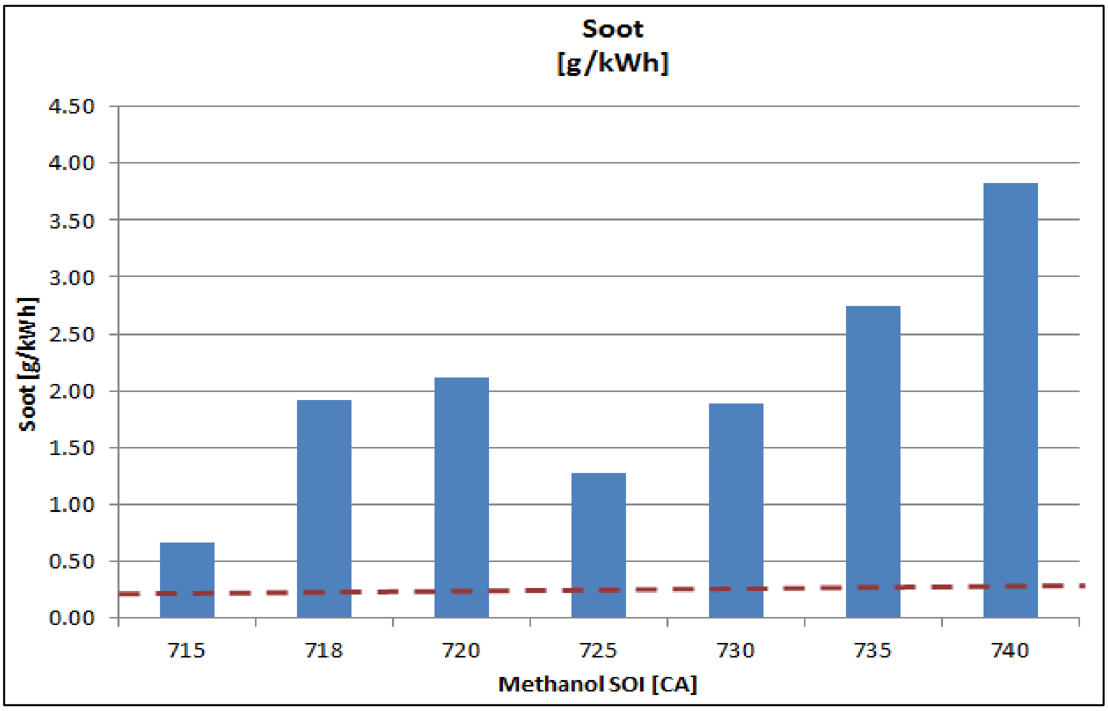


Figure 4.10 : Soot emission results for case 3.

In case 3, 0.45 methanol mass fraction cases are not successful to decrease soot emission even with various methanol SOI timings applied. Even lowest soot emission observed at 715 degree CA methanol SOI case, there is %22 percentage exceed from base diesel case as shown in Figure 4.10. As methanol SOI delayed, soot emission increases and in 740 CA, it reachs %136 percentage soot emission exceed as highest level.

Case 3 couldn't be successful in overall soot and NO emision for no EGR application. But for specific NO reduction aim, case 3 can be used and methanol injection done right after diesel injection at 714.8 CA, shows %49 NO reduction.

4.5 RCCI Cases for Various EGR Rates for Case 2

Regarding foundings in section 4.3, 718 deg CA methanol SOI is best option for getting both NO and soot reduction for case 2. In this section case 2 mixture investigated with various EGR rates to get more reduction on current parameters. Diesel SOI kept in 714.8 deg CA with 27.2 deg CA duration of injection. Methanol SOI has been kept constant at 718 deg CA with 6.5 deg CA injection duration. Case 2.b presents no EGR condition with 0.03 EGR mass fraction rate for simulating residual gasses stayed from previous cycle. %10, %15, %20, %25 EGR mass fraction rates applied, as shown in Table 4.7. 718 deg CA methanol SOI choosen from various methanol SOI cases, because it is lowest soot emission observed case. EGR affect assumed to increase soot, but decreasing NO emission simultaneously. Hence 718 deg CA selected, as it is highest NO emission, but lowest soot emission case.

Table 4.7 : RCCI cases for various EGR rates for case 2.

Case No	Diesel Amount [mg]	Methanol Amount [mg]	Diesel SOI [CA]	Diesel Duration [CA]	Methanol SOI [CA]	Methanol Duration [CA]	EGR Rate [%]
2.b	15.000	3.375	714.8	27.2	718	6.5	0.03
2.h	15.000	3.375	714.8	27.2	718	6.5	0.10
2.i	15.000	3.375	714.8	27.2	718	6.5	0.15
2.k	15.000	3.375	714.8	27.2	718	6.5	0.25
2.m	15.000	3.375	714.8	27.2	718	6.5	0.30

Corresponding to results in Figure 4.11, as much as EGR mass fraction rate increase, NO emission decrease regardingly. Moreover %30 EGR rate case providing %89 NO emission reduction from base case.

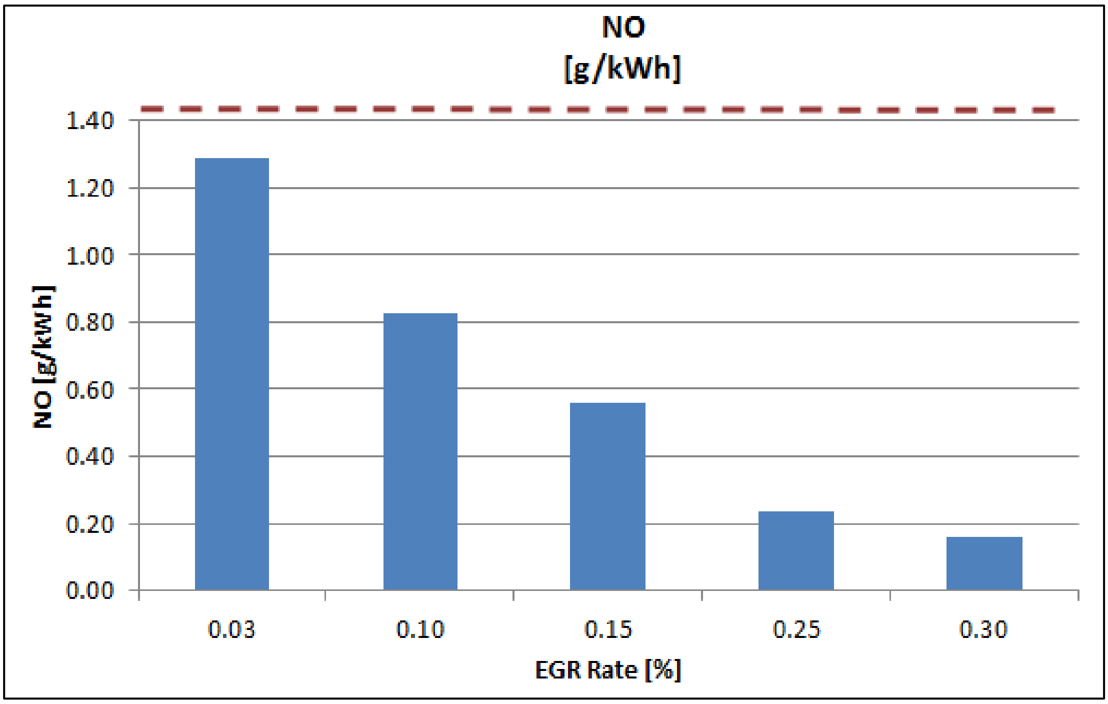


Figure 4.11 : NO emission results for case 2.

Soot emission results of case 2 with various EGR rate applications in Figure 4.12, show increase on soot mass when EGR mass fraction increased, as assumed. Case 2 with %10 EGR rate exceeds soot emission %11 from base case. Proportionally, %7 EGR could be applied to stay in border of soot limit and decrease NO simultaneously roughly %30 overall.

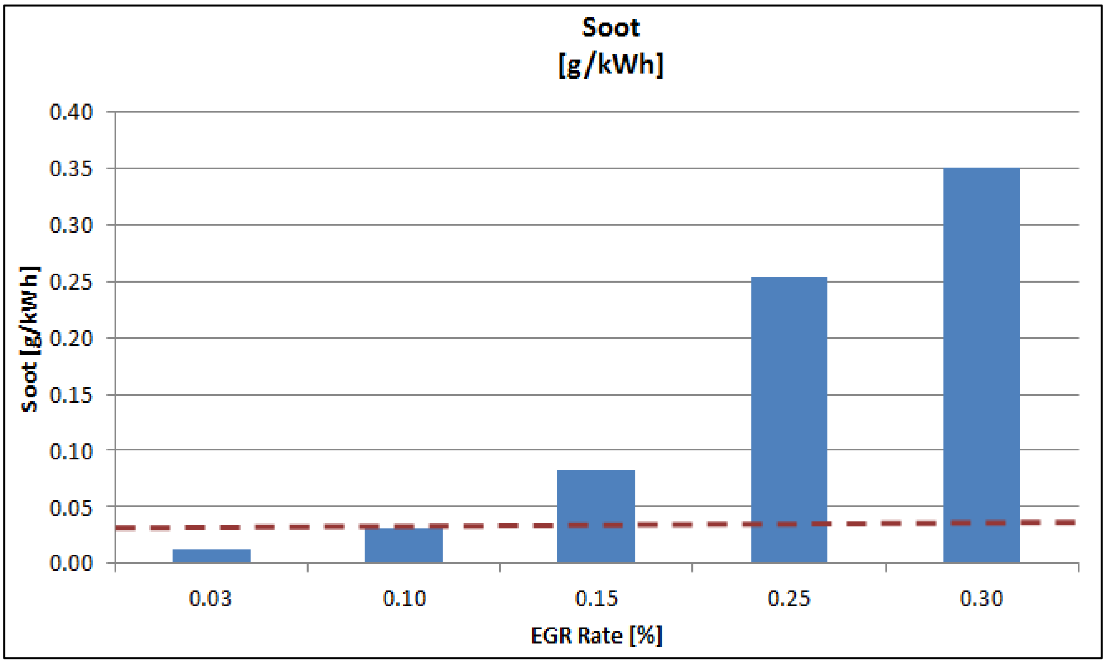


Figure 4.12 : Soot emission results for case 2.

4.6 RCCI Cases for Various EGR Rates for Case 3

In this section case 3 investigated with application of different EGR rates. Methanol mass fraction, 0.45, has not been changed. Diesel SOI kept in 714.8 deg CA with 21.7 injection duration and methanol SOI taken as 715 deg CA regarding results in Section 4.5. %10, %15, %25 EGR rates have been applied, as shown in Table 4.8. 0.03 EGR rate simulate non-EGR application. Results compared with base diesel case.

Table 4.8 : RCCI cases for various EGR rates for case 3.

Case No	Diesel Amount [mg]	Methanol Amount [mg]	Diesel SOI [CA]	Diesel Duration [CA]	Methanol SOI [CA]	Methanol Duration [CA]	EGR Rate [%]
3.a	12.000	9.823	714.8	21.7	715	18.8	0.03
3.h	12.000	9.823	714.8	21.7	715	18.8	0.10
3.i	12.000	9.823	714.8	21.7	715	18.8	0.15
3.j	12.000	9.823	714.8	21.7	715	18.8	0.25

NO emission results shown in Figure 4.13. At %10 percentage of EGR poin there is a trade off on NO emission. Increasing EGR till %10 increase NO, but more increase on EGR rate, create decrease on NO emission. Lowest NO emission with %62 reduction obtained from %25 EGR case.

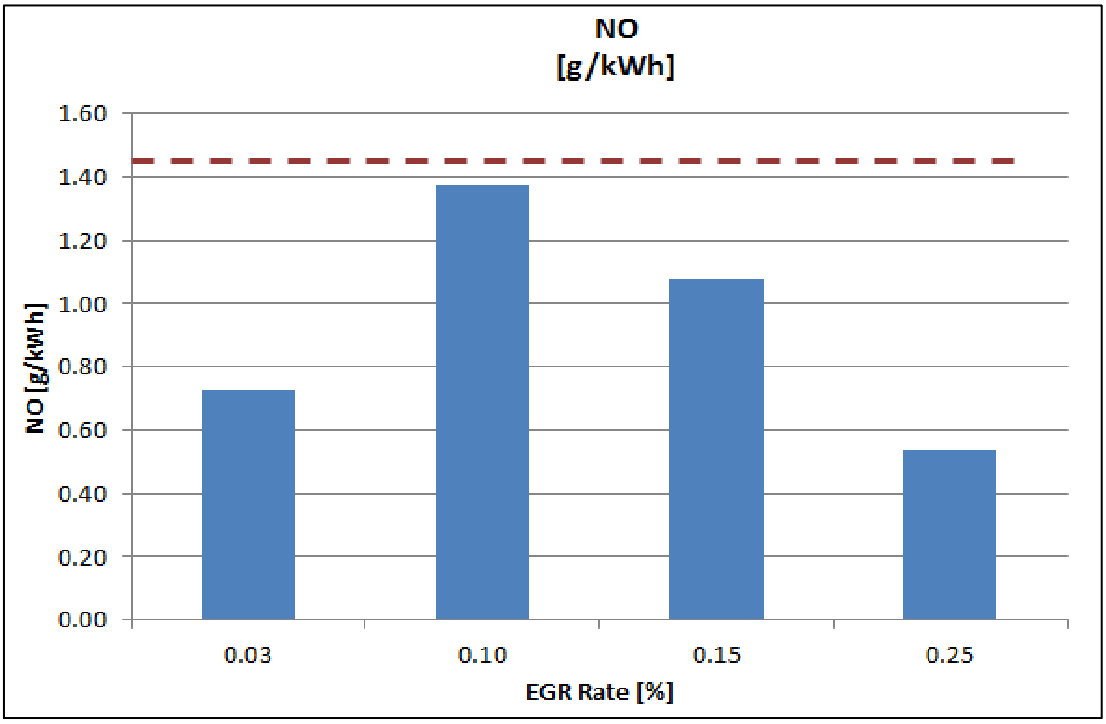


Figure 4.13 : NO emission results for case 3.

Soot results shown in in Figure 4.14. %10 EGR case provides lowest soot emission with %80 soot reduction. Rising EGR rate from %10 to %25 provides increasing soot emission, as assumed, but during that increase soot emission still stays in limits.

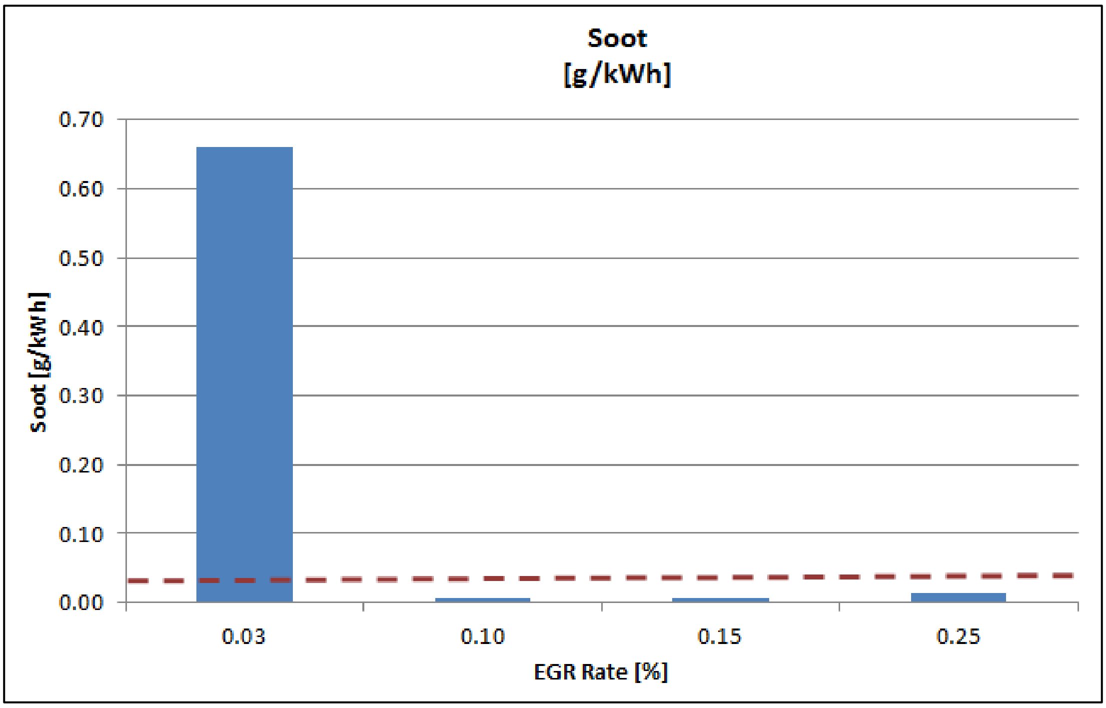


Figure 4.14 : Soot emission results for case 3.

4.7 RCCI Cases for Early Diesel and Methanol SOIs for Case 2

In Section 4.3 and 4.5, case 2 has been investigated for methanol SOI change and EGR affect. 718 deg CA found as highest NO, but lowest soot emission case which allows to use EGR and keep soot emission in limit. In Section 4.5, EGR rate that limits soot found as %7 and further EGR mass fraction rate increse, create high soot emission. In this section, increasing SOI advance of both diesel and methanol injections will be investigated for %15 EGR condition, as shown in Table 4.9. First case, 2.b kept for comparison as best case in case 2 previous results.

Table 4.9 : RCCI cases for early diesel and methanol SOIs for case 2.

Case No	Diesel Amount [mg]	Methanol Amount [mg]	Diesel SOI [CA]	Diesel Duration [CA]	Methanol SOI [CA]	Methanol Duration [CA]	EGR Rate [%]
2.b	15.000	3.375	714.8	27.2	718	6.5	0.03
2.i	15.000	3.375	714.8	27.2	718	6.5	0.15
2.j	15.000	3.375	704.8	27.2	708	6.5	0.15
2.l	15.000	3.375	704.8	27.2	700	6.5	0.15

Regarding Figure 4.16, NO emission shows decrease when %15 EGR rate added over case 2 without changing SOI. When EGR rate kept same, and both diesel and methanol SOI are taken 10 deg CA earlier, results show that NO emission increase due to increasing pressure (Figure 4.15) and temperature parameters in combustion chamber.

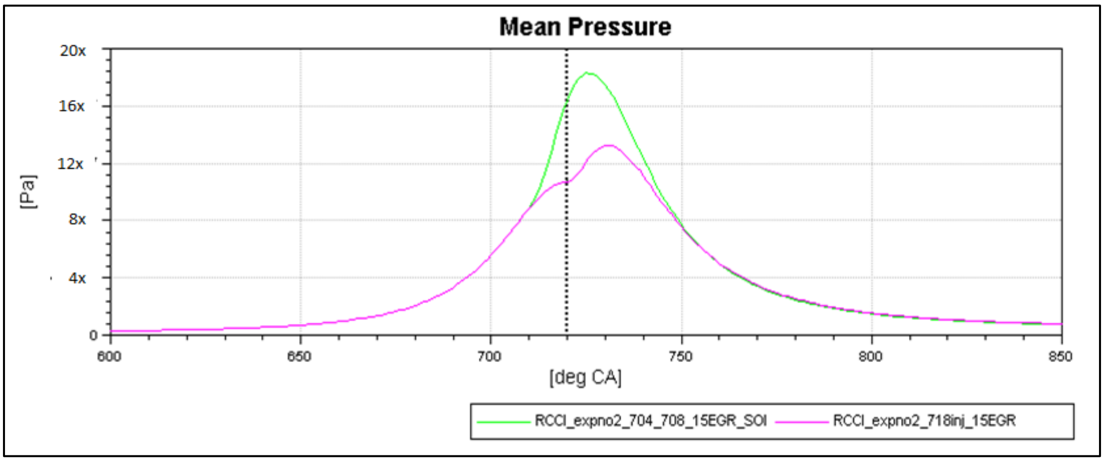


Figure 4.15 : Mean pressure for case 2.i(pink line) and 2.j(green line).

Furthermore when methanol SOI advance increased 8 degree CA more from 708, NO emission shows decrease. Results shows that methanol SOI has high influnce on NO emission in positive side when exp 2.j and 2.l compared. Without changing EGR and diesel SOI parameters, only increase on advance SOI on methanol helps to decrease NO emission with %16 percentage.

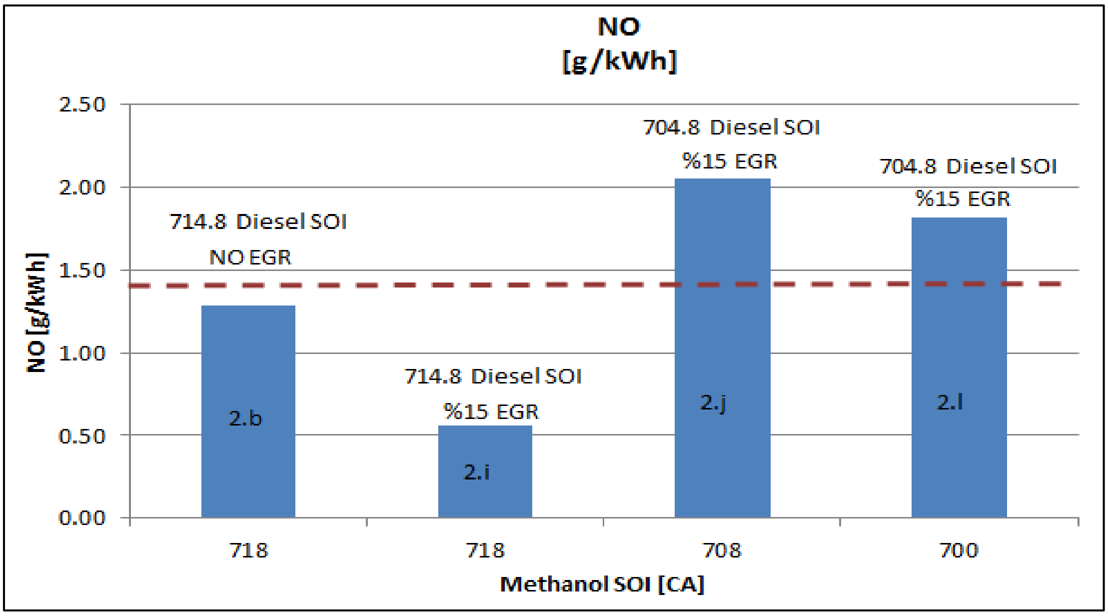


Figure 4.16 : NO emission results for case 2.

But taking diesel injection earlier cause temperature increase, even methanol SOI advance couldn’t help to decrease NO emission or keep in base case limits, as shown in Figure 4.16. In-cyclinder temperatures shown in Figure 4.17. There is no significant temperature profile difference at 760deg CA between %15 EGR rated 3 cases. But only case 2.i has less high temperatures in cylinder bowl rather than rest of two cases which could be reason for less NO mass fraction results.

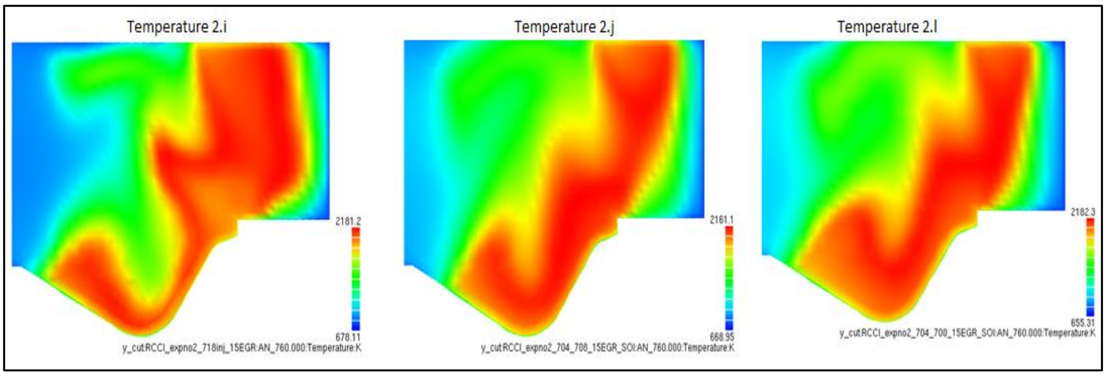


Figure 4.17: Incylinder temperatures at 760 deg CA.

Increasing advance on diesel SOI, increased NO emisison, and soot emission assumed to be reduced. But results show in Figure 4.18 that with SOI advance of diesel or methanol or both couldn’t reduce soot amount even engine indicated power increased per advance SOI case.

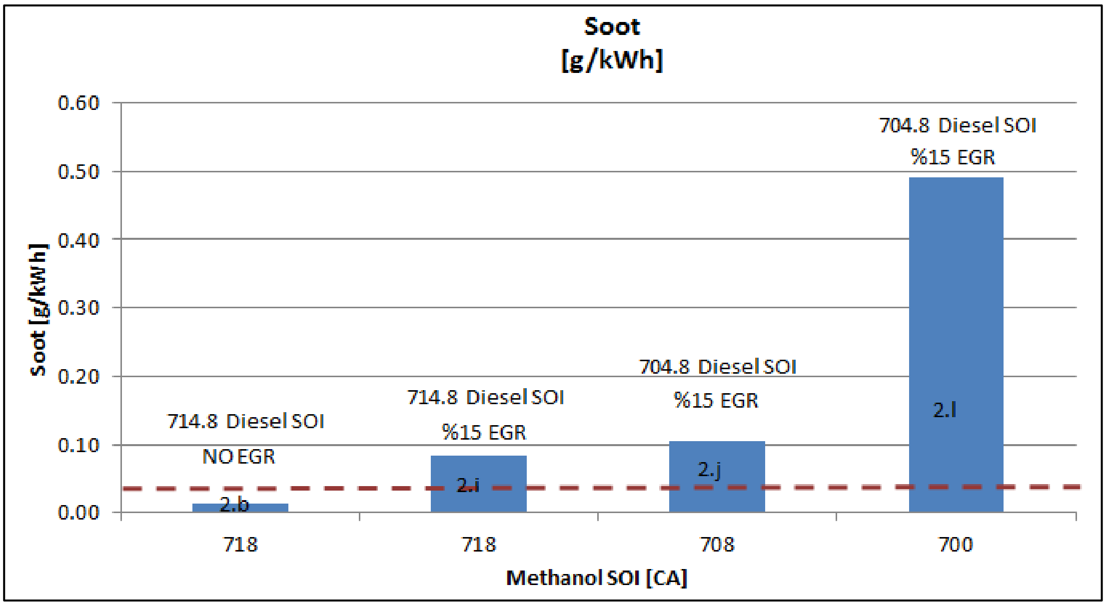


Figure 4.18 : Soot emission results for case 2.

In Figure 4.19, soot mass fraction intensity shown per %15 EGR rated 3 cases at 855 degree CA. Regarding that, soot concentration in bowl is increasing per advance on

SOI. Because earlier injected fuel stay inside of bowl during combustion and during ignition couldn't find enough air to burn with and soot occurs in that area that increase soot mass fraction.

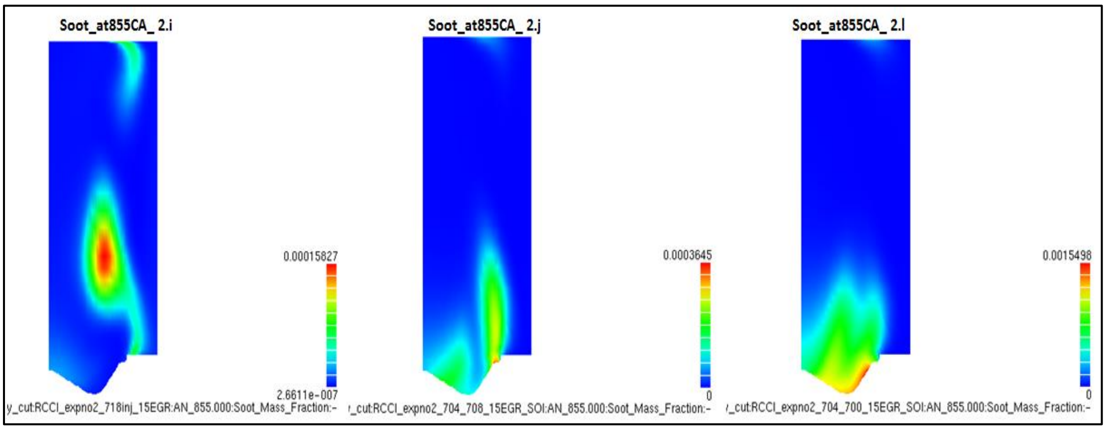


Figure 4.19 : Soot mass fraction at 855 deg CA.

4.8 RCCI Cases for Early Diesel and Methanol SOIs for Case 4

In section 4.2 regarding various mixture study results, case 4 showed %43 NO emission reduction opportunity, but it was exceeding soot emission %67 percentage from base diesel case. In this section using NO reduction opportunity of case 4, and targeting improvement on soot amount via increase advance in diesel and methanol SOI without EGR affect, will be studied. During for all 4 cases, diesel and methanol injected mass, duration, injection rate not changed, EGR taken as %3 to simulate residual gasses left from previous cycle.

In Table 4.10, 4.a shows main case 4 with 720 injection, studied in section 4.2; 4.b shows 10 deg CA advance in both methanol and diesel SOI. Case 4.c shows 5 deg CA earlier methanol SOI from case 4.b to check methanol SOI change affect withour changing diesel SOI.

Table 4.10 : RCCI cases for early diesel and methanol SOIs for case 4.

Case No	Diesel Amount [mg]	Methanol Amount [mg]	Diesel SOI [CA]	Diesel Duration [CA]	Methanol SOI [CA]	Methanol Duration [CA]	EGR Rate [%]
4.a	10.000	14.121	714.8	18.1	720	27.1	0.03
4.b	10.000	14.121	704.8	18.1	710	27.1	0.03
4.c	10.000	14.121	704.8	18.1	705	27.1	0.03
4.d	10.000	14.121	704.8	18.1	700	27.1	0.03

Regarding NO emission results in Figure 4.20, increasing SOI of both diesel and methanol 10 deg CA increased NO emission and lead to exceed base limit %17 percentage, as shown in Table 4.11. Increasing SOI advance 5 deg CA from 4.b case, increased NO %4 more from 4.b emission. Increasing methanol advance SOI 5 degree CA more, cause increase on NO emission %15 percentage from case 4.c.

Table 4.11 : Case 4 emission results.

Case No	Diesel SOI [CA]	Methanol SOI [CA]	Power [kW]	NO [g/kWh]	NO Reduction [%]	Soot [g/kWh]	Soot Reduction [%]
4.a	714.8	720	48.35	0.81	43	1.90	-6717
4.b	704.8	710	50.18	1.67	-17	5.70	-20297
4.c	704.8	705	48.88	1.74	-21	2.21	-7820
4.d	704.8	700	47.2	1.95	-36	2.18	-7717

For case 4, 0.58 mass fraction rated mixture, NO emission increase per earlier SOI conditions both for diesel and methanol injections. To stay in NO emission limit 715 deg CA methanol injection and can be done.

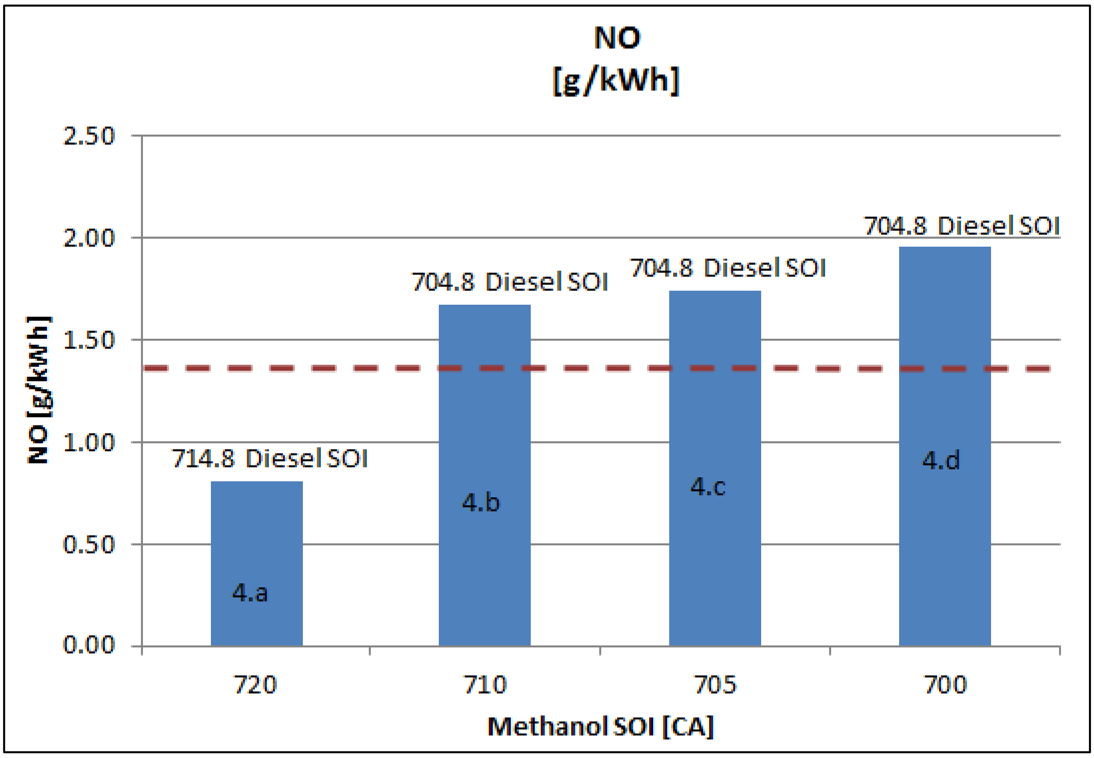


Figure 4.20 : NO emission results for case 4.

In cyclinder temperature at 760 deg CA is shown in Figure 4.22. Temperature profiles very close per 4 cases. Only first case shows different chracteristic in temperature graph, as not filling all bowl like orthers did. Figure 4.21 shows pressure change per advance on SOI. Increasing advance of diesel SOI from 714.8, creates high pressure rather than engine components can endure, which increases aging affect and may harm the engine.

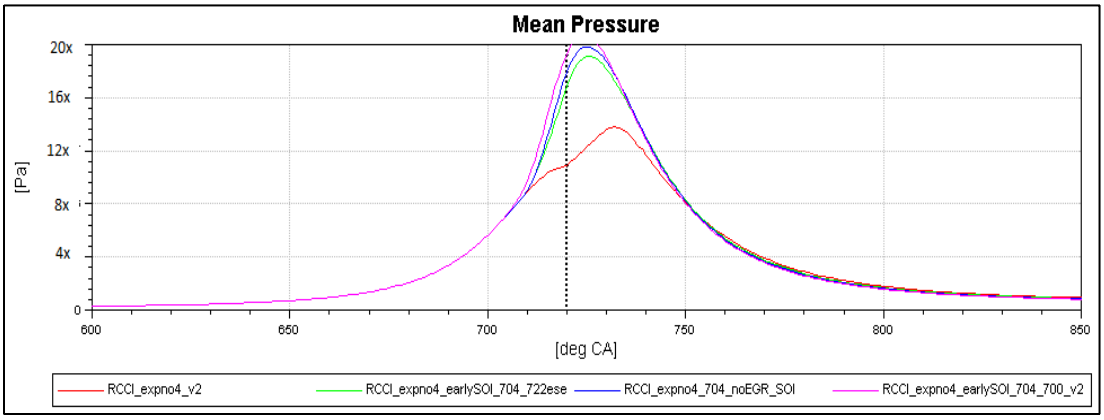


Figure 4.21 : Mean pressure for 4 cases.

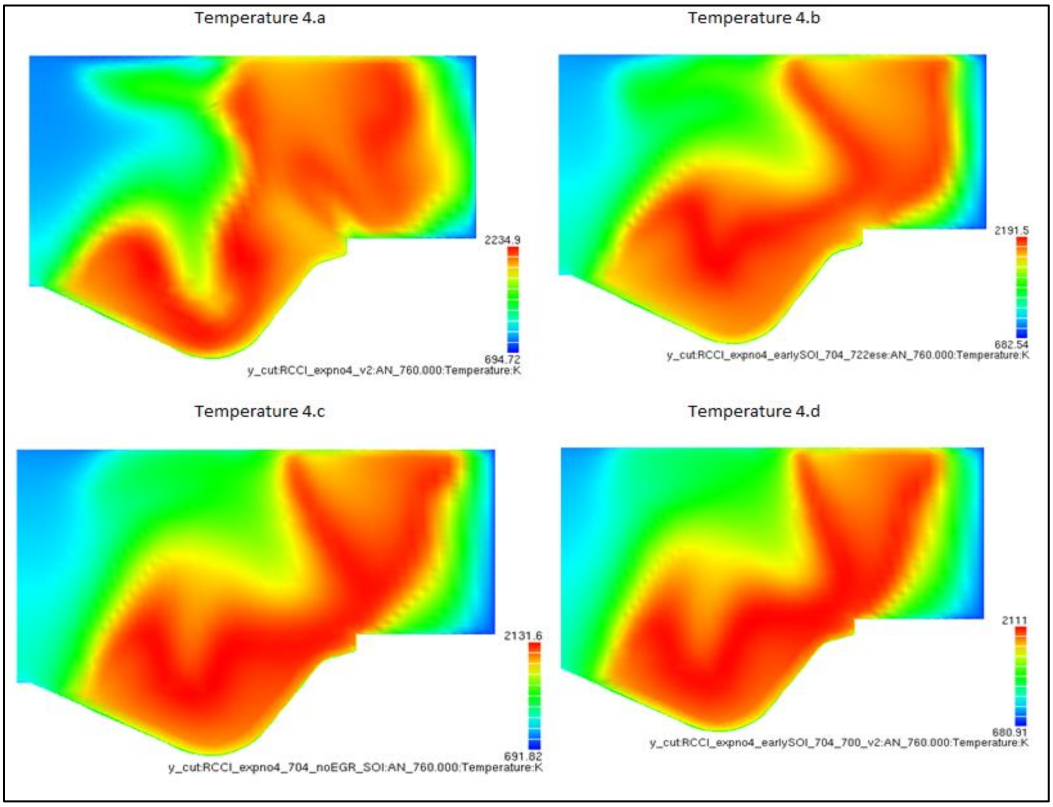


Figure 4.22 : Incylinder temperatures at 760 deg CA.

In Figure 4.16, increasing diesel and methanol SOI increase soot emission to %202 from %67, instead of improve. But critical point is when only methanol SOI advance increased 5 deg CA more, there is significant decrease %124 percentage occurs, but even that still above the limit of base case like previous section, in Figure 4.17. So with late SOI till TDC both for diesel and methanol .

So as much as injection delayed, NO mass fraction could be decreased as a result of distribution of fuel in all over cyclinder, shown in Figure 4.22. Getting injection earlier causes fuel mass gathered inner bowl and stay there during combustion process and increase NO with higher pressure (Figure 4.21) and thermal gradients (Figure 4.23) availablity. After 4.a case, all 3 cases exceed pressure limit of engine, and may cause damage on engine components.

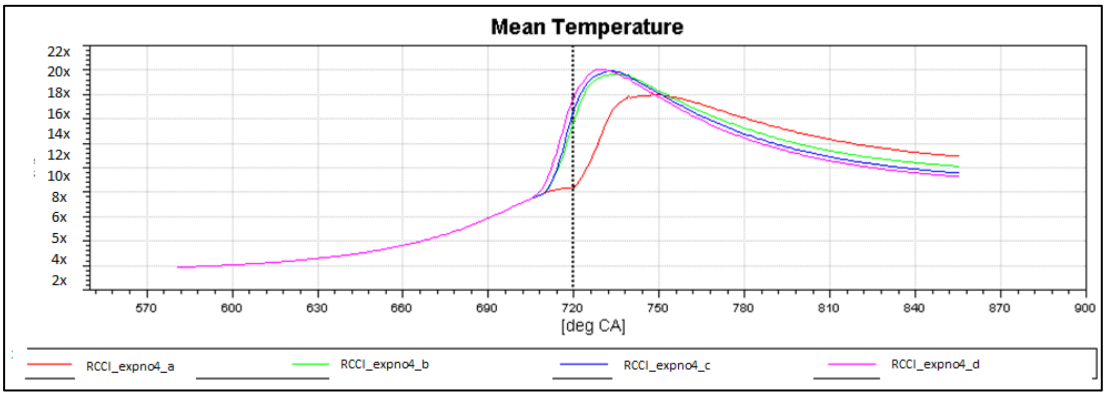


Figure 4.23 : Mean temperature for 4 cases.

About soot emission, with increase on SOI timings for diesel and methanol cause increase on soot emission as shown in Figure 4.24 and 4.25. Advance on diesel SOI cause rise on soot mass fraction with in 4.b case. There is a trade off in this point which affects soot trend during taking SOI earlier.

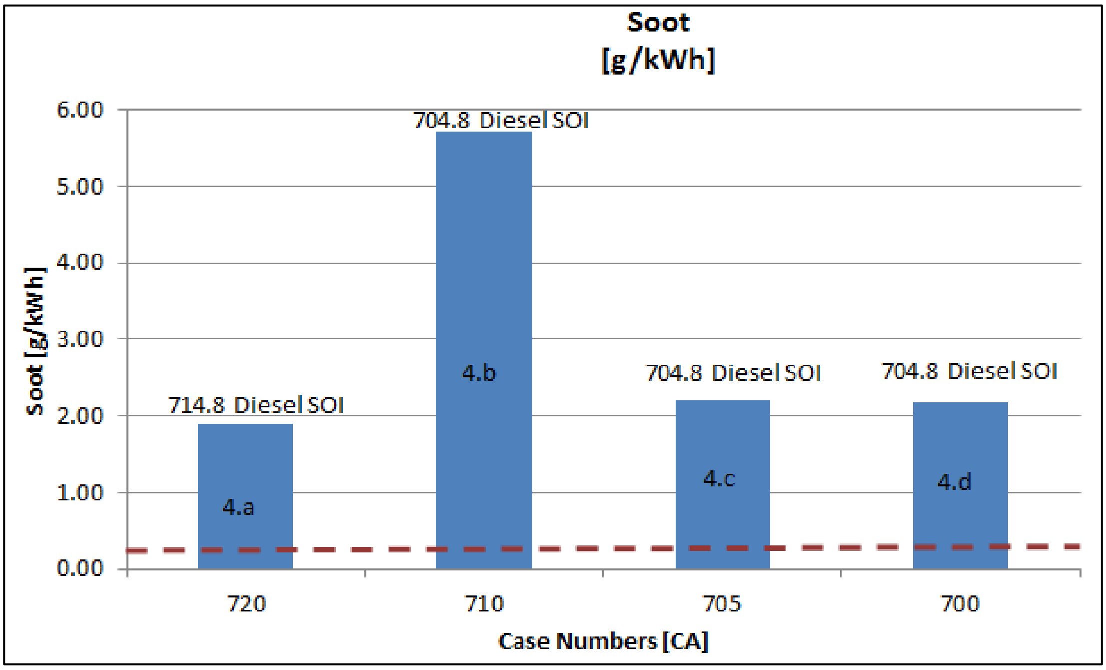


Figure 4.24 : Soot emission results for case 4.

In 710 degCA methanol and 704.8 deg CA diesel incjection, combustion efficiency falling down due to reaching critical point in diesel particules ignition. When diesel ignition starts, methanol injection cause a damp in flame progress and cause instant rise on soot mass fraction. Also in Figure 4.25, soot mass fraction distrubution could be seen as collected in inner bowl area and couldn't burn beacuse of not finding enough oxygen. As a result of insufficient combustion both diesel and methanol particules couldn't be burned and turned into unburned hydracarbons.

Methanol and diesel fuel mass fraction could be seen in Figure 4.26 and 4.27 which shows that 4.b has highest both methanol and diesel fuel mass overall at 855 deg CA.

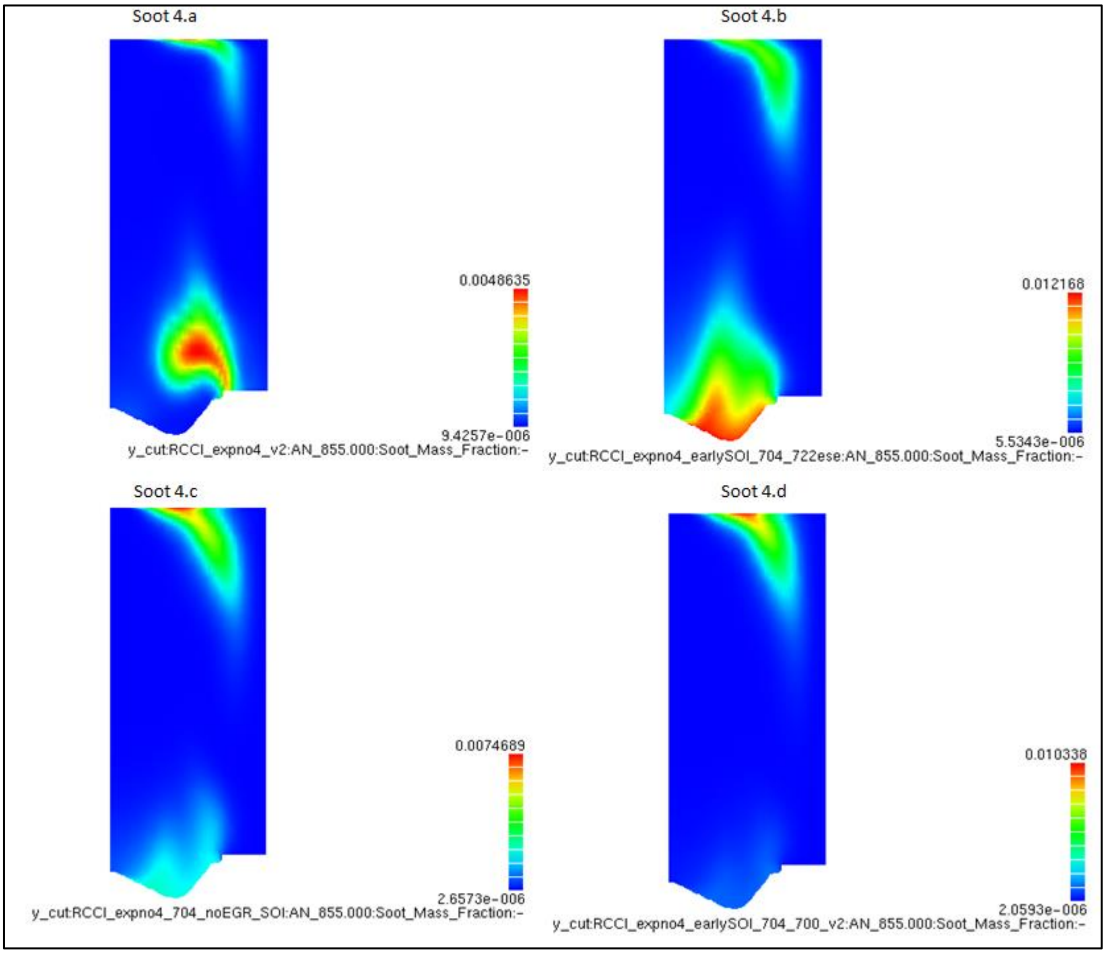


Figure 4.25 : Soot mass fraction at 855 deg CA.

For 4.c and 4.d soot results are close to each other, but 4d shows decrease on soot %1 per previous case. As also shown in Figure 4.25, hence methanol injected earlier than diesel and methanol finds enough time to mix with air, combustion improved and that helps to decrease soot emission in overall.

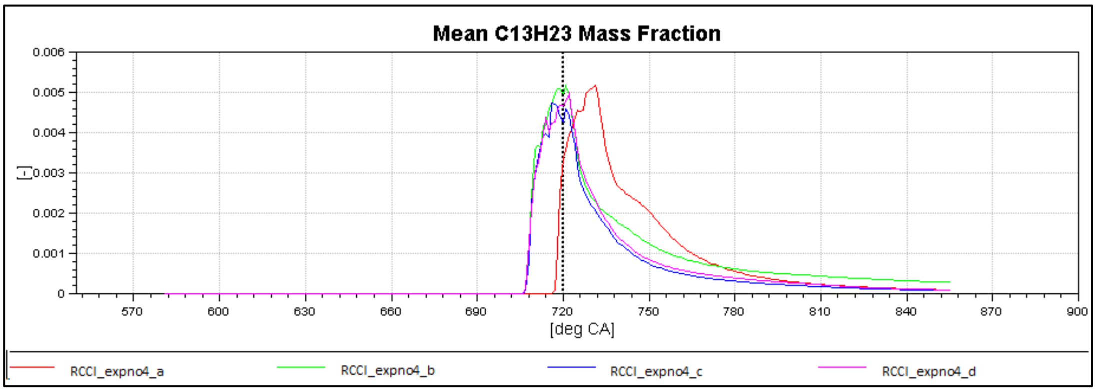


Figure 4.26 : Diesel mass fraction for 4 cases.

On the contrary 4.c and 4.d soot distribution not shown in bowl and when it's checked for fuel mass left after combustion at 850deg CA, there is less methanol and diesel mass left cylinder inside regarding Figure 4.26 and Figure 4.27.

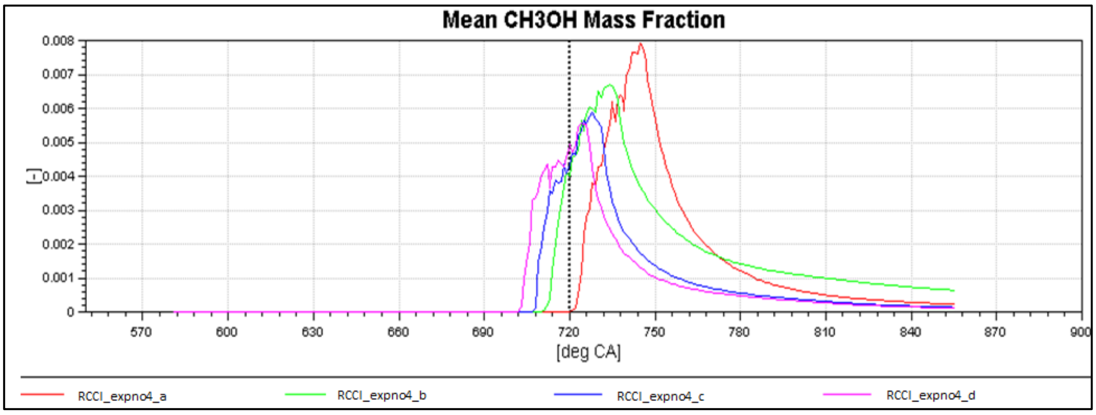


Figure 4.27 : Methanol mass fraction for 4 cases.

5. CONCLUSIONS AND RECCOMENDATIONS

RCCI engine has been studied on 32 different variants overall. These 32 runs include; different SOI timings of methanol between 700-740 degree CA, different SOI timings of diesel between 704.8-714.8 degree CA, various EGR rates between %10 to %30, 7 different methanol mass fraction rated fuel mixtures overall.

At first step created AVL Fire diesel engine model has been verified with part load engine dynometer test results. This validated model mesh cell size choosen from 5 mesh variant option, regarding sensivity of pressure, temperature, accumulated heat release, NO mass fraction, soot mass fraction results in order to achieve mesh independency, as detaily mentioned in Chapter 3.

RCCI engine results reviewed in Chapter 4, to understand behavior and charecteristics of methanol-diesel fueled RCCI engine emission and performance. During that study NO mass fraction, NO mass per kWh, soot mass fraction, soot mass per kWh, CO mass fraction, indicated power, mean incylinder pressure, mean incylinder temperature, NO and soot distrubution over combustion chamber, mean mass, diesel mass fraction in cylinder, methanol mass fraction in cylinder have been investigated and results compared with base diesel case for improvement assessment.

Regarding all cases, most problematic part was soot improvement. In 25 cases, NO emission reduced from base diesel case, but soot improvement only achieved in 6 cases.

Soot mass reduced from base diesel case (Case 1) listed in Table 5.1. Regarding results; case 2 with 0.184 methanol mass fraction and case 3 with 0.45 methanol mass fraction are both successful to achieve soot reduction. With all those cases NO emission reduction also achieved simultaneously. In 6 cases power decrease which reachs up to %7 percentage observed. NO and soot reduction percentages calculated from mass per kWh, hence indicated power decrease also calculated and even that emission decrease observed.

Table 5.1 : Soot improvement achieved RCCI cases

Case NO	Methanol Mass Fraction [-]	Diesel SOI [CA]	Methanol SOI [CA]	EGR Rate [%]	Indicated Power [%]	NO Reduction [%]	Soot Reduction [%]
1	0	714.8	-	0.03	100.00	-	-
2.a	0.184	714.8	715	0.03	96.93	12	53
2.b	0.184	714.8	718	0.03	95.87	10	54
2.c	0.184	714.8	720	0.03	95.11	16	46
3.h	0.450	714.8	715	0.10	94.61	4	80
3.i	0.450	714.8	715	0.15	94.63	25	74
3.j	0.450	714.8	715	0.25	93.94	62	51

According to priorities set, best case could be also selected.

- ❖ For lowest soot production; case 3.h can be selected, which provides %80 percentage soot reduction and %4 NO reduction in comparison to the reference diesel engine. That case have 0.45 methanol mass fraction, %10 EGR, 714.8 CA SOI of diesel, 715 CA SOI of methanol.
- ❖ For lowest NO production; case 3.j can be selected, which provides %62 NO reduction with %51 soot reduction. That case have 0.45 methanol mass fraction, %25 EGR, 714.8 CA SOI of diesel, 715 CA SOI of methanol.

In this study emisison improvement opportunities studied during all cases. In the other hand, fuel consumption could be also assest. Regarding runs with methanol mass fraction variaty provide lower fuel cost per decrease on diesel fuel amount for each cycle. For case 2 fuel amount seems increase from 16.57 mg to 18.375 mg, but diesel mass decrease from 16.57 mg to 15 mg per cycle, which is similar for case 3. That creates decrease on diesel fuel consumption, as shown in Table 5.2.

Table 5.2 : Diesel fuel consumption

Case NO	Diesel Amount [mg]	Methanol Amount [mg]	Meth. Mass Fraction [-]	Indicated Power [%]	Diesel Fuel Consumption [mg/%kW]
1	16.570	0.000	0	100	0.17
2.a	15.000	3.375	0.184	96.93	0.15
2.b	15.000	3.375	0.184	95.87	0.16
2.c	15.000	3.375	0.184	95.11	0.16
3.h	12.000	9.823	0.450	94.61	0.13
3.i	12.000	9.823	0.450	94.63	0.13
3.j	12.000	9.823	0.450	93.94	0.13

Base diesel case provides 0.17 mg/%kW diesel fuel consumption, case 2 provides 0.15-16 mg/%kW and case 3 provides 0.13 mg/%kW. As much as methanol mass fraction decreases from case 1 to case 8, diesel fuel consumption decrease per cases, when 8 different cases ,regarding variant methanol mass fraction, investigated . That results indicate that emission decrease and also fuel consumption could be gathered with methanol-diesel fuel RCCI engines.

Regarding all case runs following results could be listed;

1. In order to decrease soot emission from base diesel case, diesel fuel injection should be kept after -6 degree advance of SOI. Further increase on diesel SOI increases soot emission as a result of collected diesel fuel inside of piston bowl after injection. That leads to create rich area inside of piston bowl, and fuel could not find enough oxygen to be burned. This mechanism yields to high soot mass fraction.
2. SOI for methanol is an important parameter for the control of NO emissions. Advancing SOI, generally increases NO emissions due to high temperature and pressure gradients. However, depend on methanol mass fraction of case, there could be different results observed.
3. Increasing methanol mass fraction decreases NO emissions, but increases soot emissions.
4. Increase in EGR mass fraction, reduces NO emissions, while increasing soot emission dramatically. EGR rates higher than 30% may cause soot emission problems.

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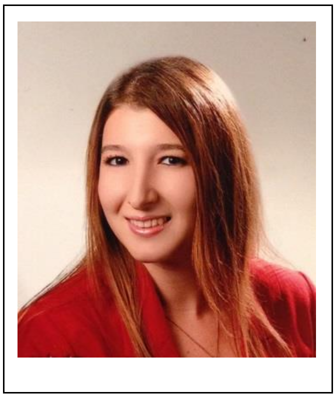
CURRICULUM VITAE



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PUBLICATIONS, PRESENTATIONS AND PATENTS ON THE THESIS:

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