

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL

PARTIALLY PREMIXED CHARGE
COMPRESSION IGNITION ENGINE OPTIMIZATION

CENGİZHAN CENGİZ

A THESIS OF DOCTORATE
MECHANICAL ENGINEERING DEPARTMENT

ADVISOR: DR. SALİH ÖZEN ÜNVERDİ

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T.C.
GEBZE TEKNİK ÜNİVERSİTESİ
LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

KISMI ÖN KARIŞIM DOLGULU
SIKIŞTIRMA ATEŞLEMELİ MOTOR
OPTİMİZASYONU

CENGİZHAN CENGİZ

DOKTORA TEZİ
MAKİNA MÜHENDİSLİĞİ ANABİLİM DALI

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To my Family.

ABSTRACT

The main subject of this thesis is to investigate the PCCI (Premixed Charge Compression Ignition) combustion phenomenon in HDDI (Heavy Duty Direct Injection) diesel engines by experiments and CRFD (Computational Reactive Fluid Dynamics) simulations. It is aimed to improve the understanding of PCCI combustion mode by analyzing the spray penetration, mixture formation and combustion characteristics of the diesel fuel injected into the combustion chamber, to integrate this combustion mode into the conventional diesel engines to reduce engine-out harmful emissions without causing a negative impact on engine performance and fuel efficiency at part load.

To reduce NO_x (nitrogen oxide) and soot emissions during the operation of an HDDI diesel engine mass-produced by Ford Otosan in diesel and PCCI combustion modes at low loads, the effects of injection timing, multiple injection strategies and EGR (Exhaust Gas Recirculation) on the performance and emission characteristics of a single-cylinder research engine have been investigated through experimental and computational studies. The main finding of the experimental study is that in part-load engine operation, a double injection strategy with a heavy EGR rate may significantly reduce the spray wall impingement problem and enable delayed low-temperature combustion by improving the fuel vapor-air mixture homogeneity, which in turn reduces engine-out NO_x and soot emissions and even ISFC (Indicated Specific Fuel Consumption).

The fuel spray dynamics in the combustion chamber, auto-ignition of the resulting mixture, flame propagation and emissions formation were studied by reactive CRFD simulations. First, the computational model is validated by the engine measurements. To achieve low engine-out NO_x and soot emissions without compromising ISFC, the detailed effects of injection timing and spray inclusion angle on fuel spray penetration into the combustion chamber, in-cylinder mixture formation, spray-cylinder wall interactions, auto-ignition and PCCI combustion in a single-cylinder research engine with a stepped-lip piston bowl have been determined by CFRD simulations. Then, in the base and early intake valve opening events, the effectiveness of a split injection strategy with EGR in improving the mixture homogeneity and combustion phasing was evaluated. It is concluded that low NO_x and soot emissions can be obtained by an optimum combination of the start of injection timing and spray inclusion angle according to engine load by improving in-cylinder mixture formation and preventing spray wall impingement significantly. Furthermore, swirl-assisted combustion following split injection with heavy EGR can considerably reduce fuel spray wetting of cylinder walls and engine-out NO_x and soot emissions. On the other hand, while EIVC (Early Intake Valve Closing) theoretically improves the indicated efficiency due to effectively delayed combustion, in practice, it may lead to poor fuel atomization and in-cylinder mixture formation, incomplete combustion, elevated soot and CO (carbon monoxide) emissions, and reduced indicated efficiency.

Finally, a very advanced split injection having a suitable spray inclusion angle and a heavy EGR rate strategy under sufficient swirl may reduce engine-out NO_x and soot emissions without compromising engine performance by eliminating adverse effects of spray impingement on cylinder walls in part load operation of a DI diesel engine.

Keywords: Diesel Engine, Combustion, Injection, PCCI, EGR, NO_x, Soot, CO.

ÖZET

Bu tezin ana konusu, AHDE (ağır hizmet veren doğrudan enjeksiyonlu) dizel motorlarda ÖKSA (Ön Karışım Sıkıştırarak Ateşlemeli) yanma olayını deneyler ve HRAD (Hesaplamalı Reaktif Akışkanlar Dinamiği) simülasyonları ile araştırmaktır. Kısmi yükte motor performansı ve yakıt verimliliği üzerinde olumsuz bir etkiye neden olmadan motor çıkışında zararlı emisyonları azaltmak için geleneksel dizel motorlara ÖKSA yanma modunu entegre etmek amacıyla, yanma odasına püskürtülen dizel yakıtın nüfuziyeti, karışım oluşumu ve yanma özelliklerini analiz ederek bu modun anlaşılmasını geliştirmek amaçlanmıştır.

Ford Otosan'ın seri olarak ürettiği bir AHDE dizel motorun düşük yüklerde dizel ve ÖKSA yanma modlarında çalışması esnasında NO_x (azot oksit) ve kurum emisyonlarını azaltmak amacıyla, tek silindirli bir araştırma motorunun performans ve emisyon özelliklerine püskürtme zamanlaması, çoklu püskürtme stratejisi ve EGGB'nin (Egzoz Gazı Geri Besleme) etkileri deneysel ve hesaplamalı çalışmalarla araştırılmıştır. Deneysel çalışmanın temel bulgusu, kısmi yükte motor çalışmasında yüksek EGGB oranına sahip çift püskürtme stratejisinin püskürtülen yakıtın silindir duvarlarına çarpma problemini önemli ölçüde azaltabileceği ve yakıt buharı-hava karışımı homojenliğini artırarak gecikmeli düşük sıcaklıkta yanmaya olanak verebileceği, sonuçta motor çıkışında NO_x ve kurum emisyonlarını ve hatta motorun BÖYT'ni (belirtilen özgül yakıt tüketimi) azaltabileceğidir.

Yanma odasına püskürtülen yakıtın dinamiği, oluşturulan karışımın kendiliğinden tutuşması, alevlerin yayılması ve emisyon oluşumu reaktif HRAD simülasyonları ile incelenmiştir. Önce hesaplamalı model motor ölçümleriyle doğrulanmıştır. BÖYT'nden ödün vermeden motor çıkışında düşük NO_x ve kurum emisyonları elde etmek için, enjeksiyon zamanlaması ve püskürtme içerme açısının, kademeli dudaklı piston çanaklı tek silindirli bir araştırma motorunda püskürtülen yakıtın yanma odasına nüfuzu ve silindir duvarları ile etkileşimleri, silindir içi karışım oluşumu, otomatik ateşleme ve ÖKSA yanması üzerindeki ayrıntılı etkileri, HRAD simülasyonları ile belirlenmiştir. Ardından, baz ve erken emme valfi açma olaylarında, EGGB'li bölünmüş yakıt püskürtme stratejisinin karışım homojenliğini ve yanma fazını iyileştirme üzerindeki etkinliği değerlendirilmiştir. Motor yüküne göre değişen püskürtme başlangıcı zamanlaması ve püskürtme içerme açısının optimum kombinasyonu ile silindir içi karışım oluşumunu iyileştirerek ve püskürtülen yakıtın duvar çarpmasını önemli ölçüde önleyerek düşük NO_x ve kurum emisyonlarının elde edilebileceği sonucuna varılmıştır. Ayrıca, ağır EGGB'li ortama yakıtın bölünerek püskürtülmesinin ardından gerçekleşen silindir ekseni etrafında girdap destekli yanma, yakıtın silindir duvarlarını ıslatmasını ve motor çıkışında NO_x ve kurum emisyonlarını önemli ölçüde azaltabilir. Öte yandan, EEVK (Erken Emme Valfi Kapama), teorik olarak etkili bir şekilde gecikmiş yanma nedeniyle belirtilen verimliliği artırırken, pratikte yakıt atomizasyonu ve silindir içinde karışım oluşumunda sorunlara, eksik yanmaya, kurum ve CO emisyonlarının artmasına ve belirtilen verimliliğin azalmasına neden olabilir.

Son olarak, kısmi yükte çalışan bir DI dizel motorda silindir ekseni etrafında yeterli girdap hareketi altında uygun bir püskürtme açısıyla çok erken bir bölünmüş püskürtme ve ağır bir EGGB oranı stratejisi yakıtın silindir duvarlarına çarpmasını önleyerek motor performansından ödün vermeden NO_x ve kurum emisyonlarını azaltabilir.

Anahtar Kelimeler: Dizel Motor, Yanma, Enjeksiyon, ÖKSA, EGGB, NO_x , Kurum, CO.

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LIST OF SYMBOLS AND ABBREVIATIONS

Q_{net}	: Net Heat Release, Joule
Q_{ch}	: Chemical Heat Release, Joule
Q_{ht}	: Heat exchanged by the gas from cylinder
t	: Time, second
V	: Volume, m ³
γ	: Ratio of specific heat capacities
p	: Pressure, Pa
θ	: Crank Angle, degree
ϕ	: Equivalence Ratio
EGR_{rate}	: EGR rate
$[NO_x]_{intake}$	: Intake NO _x mass concentration
$[NO_x]_{exh.}$	: Exhaust NO _x mass concentration
$\dot{m}$	: Mass flow rate, kgs ⁻¹
R	: Ideal gas constant, Jkg ⁻¹ K ⁻¹
T	: Absolute Temperature, K
η_v	: Volumetric Efficiency, -
η_i	: Indicated Efficiency
$\rho_{exhaust}$	: Exhaust Gas Density, kgm ⁻³
P_{engine}	: Engine power, W
$\dot{m}_{exhaust}$	: Exhaust mass flow rate, kgh ⁻¹
ρ	: Density
u_i	: Velocity component in ith cartesian direction, ms ⁻¹
x_i	: Cartesian coordinate in ith direction, m
S	: Source term
σ_{ij}	: Stress tensor, Pa
μ	: Viscosity, Pas
δ_{ij}	: Kronecker delta
e	: Specific internal energy, Jkg ⁻¹
K	: Sum of molecular and turbulent thermal conductivities, Wm ⁻¹ K ⁻¹
Y_m	: Mass fraction of species m, -
h_m	: Specific enthalpy of species m, Jkg ⁻¹
c_p	: Specific heat capacity at constant pressure, Jkg ⁻¹ K ⁻¹
c_v	: Specific heats capacity at constant volume, Jkg ⁻¹ K ⁻¹
D	: Mass diffusion coefficient, m ² s ⁻¹
k	: Turbulent kinetic energy, Jkg ⁻¹
ε	: Dissipation rate of turbulent kinetic energy, Jkg ⁻¹ s ⁻¹
τ_{ij}	: Reynolds stress tensor, Pa
Pr_k	: Prandtl number, -
C_s	: Constant
S_{ij}	: Mean strain rate tensor, s ⁻¹
N_p	: Number of drops, -
$F_{drag,i}$	: Drag force in ith cartesian direction, N
A	: Total number of chemical species, -
$v'_{m,r}$	: Stoichiometric coefficients for the reactants and products
L	: Total number of elementary reactions, -
χ_m	: Chemical symbol for species m.

$\dot{\omega}_m$	: Net volumetric production rate of species m, $\text{molm}^{-3}\text{s}^{-1}$
q_r	: Rate-of-progress parameter
k_{fr}	: Forward reaction rate coefficients
k_{rr}	: Reverse reaction rate coefficients
A_r	: Pre-exponential factor
E_r	: Activation energy, Jmol^{-1}
R_u	: Universal Gas Constant, $\text{Jmol}^{-1}\text{K}^{-1}$
$\bar{h}_m$	: Molar specific enthalpy, Jmol^{-1}
X_m	: Mass fraction of species of m, -
A_{sf}	: Pre-exponential factor for soot-formation kinetics
A_{so}	: Scaling factor of NSC soot oxidation kinetics
NO_x	: Nitrogen oxides
EU	: European Union
U.S.	: United States
EPA	: Environmental Protection Agency
VECTO	: Vehicle Energy Consumption Calculation Tool
CO_2	: Carbon Dioxide
LLC	: Low Load Cycle
RDE	: Real Driving Emissions
ATS	: After Treatment System
PM	: Particulate matter
EGR	: Exhaust Gas Recirculation
DPF	: Diesel Particle Filter
DI	: Direct Injection
SCR	: Selective Catalytic Reduction
CO	: Carbon monoxide
UHC	: Unburnt Hydrocarbon Emissions
DOC	: Diesel Oxidation Catalyst
LTC	: Low Temperature Combustion
HCCI	: Homogenous Charge Compression Ignition
RCCI	: Reactivity Controlled Compression Ignition
PCCI	: Premixed Charge Compression Ignition
CDC	: Conventional Diesel Combustion
CI	: Compression Ignition
CFD	: Computational Fluid Dynamics
EIVC	: Early Intake Valve Closing
SOI	: Start of Injection
SI	: Spark Ignited
WLTC	: Worldwide Harmonized Light Vehicles Test Cycle
AHRR	: Apparent Heat Release Rate, W
OH	: Hydroxyl Radical
NO	: Mono-nitrogen oxide
N_2O	: Dinitrogen monoxide
O_2	: Oxygen
PAH	: Poly-aromatic Hydrocarbons
C_2H_2	: Acetylene
C_3H_3	: Cyclopropenium
C_6H_6	: Benzene
MAH	: Mono-Aromatic Hydrocarbons
H_2O	: Water

MK	: Modulated Kinetics
TDC	: Top Dead Centre
CR	: Compression Ratio, -
UNIBUS	: UNiform BULky combustion System
ATDC	: After Top Dead Center
MULDIC	: MULTiple stage Diesel Combustion
HiMICS	: Homogenous charge intelligent Multiple Injection Combustion System
PREDIC	: PREmixed Diesel Combustion
HDDI	: Heavy Duty Direct Injection
BDC	: Bottom Dead Center
IMEP	: Indicated Mean Effective Pressure, bar
MFB50%	: 50% Mass Fraction Burned, °CA BTDC
CE	: Combustion Efficiency, -
FTIR	: Fourier Transform Infrared Spectroscopy
FSN	: Filtered Smoke Number
DIS	: Double Injection Strategy
SMIS	: Single Main Injection Strategy
SPI	: Single Pilot Injection
SMI	: Single Main Injection
BMEP	: Brake Mean Effective Pressure, bar
AFR	: Air to Fuel Ratio, kg air/kg fuel
HRR	: Heat Release Rate, W
SOIgn	: Start of Ignition, °CA BTDC
ID	: Ignition Delay, °CA
DCC	: Diffusion-Controlled Combustion
ASI	: Advanced Start of Injection
ICP	: In-cylinder Pressure, bar
CA	: Crank Angle, °
FRP	: Fuel Rail Pressure, bar
MPRR	: Maximum Pressure Rise Rate, bar/°CA
BTDC	: Before Top Dead Center
ISFC	: Indicated Specific Fuel Consumption, g/kW
TIS	: Triple Injection Strategy
CD	: Combustion Duration, °CA
FVAM	: Fuel vapor air mixture
PCHTE	: Product of Combustion and Heat Transfer Efficiencies, -
HTE	: Heat Transfer Efficiency, -
CCE	: Closed Cycle Efficiency, -
RANS	: Reynolds Average Navier Stokes
RNG	: Renormalization Group
NTC	: No-time Collision
AFVM	: Air fuel vapor mixture
AMR	: Adaptive Mesh Refinement
n-C ₇ H ₁₆	: N-heptane
C ₁₄ H ₃₀	: Tetradecane
NSC	: Nagle and Strickland-Constable
RER	: Reaction equivalence ratio
STPL	: Spray tip penetration length, m
PLIF	: Planar Laser-Induced Fluorescence

SIA : Spray Inclusion Angle, degrees
ESI : Early Single-Injection
CoC : Center of combustion



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1. INTRODUCTION

1.1. Introduction

There are various proposed solutions to reduce problems related to combustion in heavy-duty CI engines in the previous section. These solutions include using multiple injection strategies, optimizing fuel rail pressure, reducing compression ratio, optimizing EGR rate, utilizing narrow spray inclusion angle injectors, controlling intake temperature, and optimizing intake valve closing timing. However, there is currently no widely used commercial application of PCCI combustion in the automotive industry, and further research and technology development are needed to apply this type of combustion. The motivation of the thesis is to set-up, analyze and optimize PCCI combustion in heavy-duty DI diesel engines by experiments and CFD simulations, and introduce effective methods for reducing NO_x and soot emissions that can be applied in commercial applications.

DI diesel engines are a popular choice for heavy-duty vehicles due to their impressive thermal efficiency, durability, and dependability compared to spark ignited gasoline engines. However, they have drawbacks associated with higher nitrogen oxides (NO_x) and soot emissions compared to gasoline engines. The formation of NO_x and soot emissions in DI diesel engines is influenced by various factors, including the spray characteristics of the fuel, the combustion process, and the engine design. These emissions are harmful to human health and the environment, and have been linked to respiratory diseases, cancer, and global warming [1], [2]. The reduction of NO_x and soot emissions resulting from IC engine chemical reactions is of paramount importance in addressing the associated health and environmental impacts. Consequently, exhaust emission regulations have been implemented within the automotive industry for a long time with the aim of achieving significant reductions in these emissions. It is evident that complying with the rigorous emission standards of the European Union (EU), the United States (U.S.) Environmental Protection Agency (EPA), and forthcoming regulations such as EU7 and EPA2027 would pose significant challenges due to the significant levels of NO_x and soot emissions produced by diesel

engines. The present status of the EU and U.S. regulations for heavy duty compression ignition engines are given in **Figure 1.1** and **Figure 1.2** respectively [3], [4].

Stage	Date	Test	CO	HC	NOx	PM	PN	Smoke
			g/kWh				1/kWh	1/m
Euro I	1992, ≤ 85 kW	ECE R-49	4.5	1.1	8.0	0.612		
	1992, > 85 kW		4.5	1.1	8.0	0.36		
Euro II	1996.10		4.0	1.1	7.0	0.25		
	1998.10		4.0	1.1	7.0	0.15		
Euro III	1999.10 EEV only	ESC & ELR	1.5	0.25	2.0	0.02		0.15
	2000.10		2.1	0.66	5.0	0.10 ^a		0.8
Euro IV	2005.10		1.5	0.46	3.5	0.02		0.5
Euro V	2008.10		1.5	0.46	2.0	0.02		0.5
Euro VI	2013.01	WHSC	1.5	0.13	0.40	0.01	8.0×10 ¹¹	

^a PM = 0.13 g/kWh for engines < 0.75 dm³ swept volume per cylinder and a rated power speed > 3000 min⁻¹

Figure 1.1: EU emission standards for heavy duty compression ignition engines.

Year	CO	HC ^a	HC ^a +NOx	NO _x	PM	
					General	Urban Bus
1974	40	-	16	-	-	-
1979	25	1.5	10	-	-	-
1985	15.5	1.3	-	10.7	-	-
1988	15.5	1.3 ^b	-	10.7 ^d	0.60	-
1990	15.5	1.3 ^b	-	6.0	0.60	-
1991	15.5	1.3 ^c	-	5.0	0.25	0.25 ^f
1993	15.5	1.3 ^c	-	5.0	0.25	0.10
1994	15.5	1.3 ^c	-	5.0	0.10	0.07
1996	15.5	1.3 ^c	-	5.0 ^e	0.10	0.05 ^g
1998	15.5	1.3	-	4.0	0.10	0.05 ^g
2004 ⁱ	15.5	-	2.4 ^h	-	0.10	0.05 ^g
2007	15.5	0.14 ^j	-	0.20 ^j	0.01	-
2024 ^k	15.5	0.14	-	0.05	0.005	-
2027 ^k	15.5	0.14	-	0.02	0.005	-
2027	6.0	0.06	-	0.035 ^l	0.005	-

a. NMHC for 2004 and later standards
b. For methanol-fueled engines, the standard is for total hydrocarbon equivalent (THCE).
c. California: NMHC = 1.2 g/bhp-hr, in addition to the THC limit.
d. California: NOx = 6.0 g/bhp-hr
e. California: Urban bus NOx = 4.0 g/bhp-hr
f. California standard 0.10 g/bhp-hr
g. In-use PM standard 0.07 g/bhp-hr
h. Alternative standard: NMHC+NOx = 2.5 g/bhp-hr and NMHC = 0.5 g/bhp-hr
i. Under the 1998 Consent Decrees, several manufacturers supplied 2004 compliant engines from October 2002.
j. NOx and NMHC standards were phased-in on a percent-of-sales basis: 50% in 2007-2009 and 100% in 2010. Most manufacturers certified their 2007-2009 engines to a NOx limit of about 1.2 g/bhp-hr, based on a fleet average calculation.
k. California only, not applicable at the federal level.
l. A NOx compliance allowance of 0.015 g/bhp-hr is added to the standard for any *in-use testing* of Medium HDE and Heavy HDE

Figure 1.2: U.S. EPA & California emission standards for heavy duty compression ignition engines, FTP, g/bhp·hr.

As per the forthcoming EU emission regulations based on Vehicle Energy Consumption Calculation Tool (VECTO), there is a limit on fuel consumption and carbon dioxide (CO₂) emissions. It is mandatory for heavy-duty vehicles to comply

with a 15% reduction in CO₂ emissions based on the average fleet average of the vehicles in 2019 [5]. Moreover, to comply with the regulations such as Low Load Cycle (LLC) or Real Driving Emissions (RDE) cycle consisting of realistic urban, rural and motorway driving conditions including cold-start, low load and stop and go operations for on-road emissions testing, novel combustion and regenerative After Treatment System (ATS) emission-control technologies are required [6], [7].

The application of advanced technologies in the automotive industry has been driven by the need to address the environmental concerns associated with diesel engines. Diesel fueled engines has been a concern due to their high emissions of NO_x and particulate matter (PM), which are harmful to environment and human health. To mitigate these effects, various technologies have been studied and applied to serial production engines to reduce emissions and increase thermal efficiency.

One of the most widely used technologies is Exhaust Gas Recirculation (EGR), which recirculates part of the exhaust gases into the intake manifold to reduce NO_x emissions. In the past, hot high-pressure EGR was used, but now, high-pressure cooled-EGR has become the standard due to its effectiveness in reducing NO_x emissions and increasing thermal efficiency. The proposed technology involves utilizing both low and high-pressure EGR on heavy-duty engines, which can further reduce emissions and improve fuel efficiency. However, the use of EGR has its limitations. One of the major drawbacks is an increase in soot production due to much richer combustion in the chamber. This has led to the development of Diesel Particle Filter (DPF), which are designed to trap and eliminate soot particles from the exhaust gases. DPF is a proven technology to restrain more than 99.9% of PM emissions and is widely used in diesel engines. Additionally, the implementation of high efficiency turbochargers and up to 3000 bars pressure common rail injection systems, coupled with direct injection (DI), has been shown to be successful in reducing both soot production and fuel consumption. Furthermore, increase of peak firing pressure limit and compression ratio of the engine have begun to be applied to obtain higher efficiency, and mitigate CO₂ emission. During engine cold start and even in low load operation, the temperatures of the ATS are not adequate for effective reduction of NO_x. To address this challenge, it is recommended to increase the exhaust gas temperature by adopting a richer and retarded combustion approach, which can enhance the efficiency of selective catalytic reduction (SCR) in reducing NO_x. Additionally, to further reduce

engine-out NO_x emissions, it is suggested to apply higher EGR rates [8]. The methods in question have only a modest capacity for reducing NO_x emissions and utilizing them can lead to penalties of increased fuel consumption and the production of excessive soot, carbon monoxide (CO), and unburnt hydrocarbon (UHC) emissions. However, diesel oxidation catalyst (DOC), DPF, and SCR of ATS is highly effective at oxidizing CO, UHC, and soot emissions, as well as diminishing NO_x levels above required light-off temperatures [9]. Therefore, under cold start and low load conditions low temperature combustion (LTC) concepts can be utilized by simultaneously reducing engine-out NO_x and soot emissions [10], [11].

Furthermore, innovative LTC techniques of Homogenous Charge Compression Ignition (HCCI), Reactivity Controlled Compression Ignition (RCCI), and Premixed Charge Compression Ignition (PCCI) have been suggested to reduce NO_x and soot emissions in such circumstances, and to reduce use of aftertreatment system [12].

HCCI combustion enables well mixed lean mixture, resulting in low NO_x emissions and efficiency levels comparable to conventional diesel combustion (CDC). However, to address CO and UHC emissions, aftertreatment technologies are necessary [13]. Moreover, elevated levels of pre-ignition and knock arise under higher engine loads, difficulties of combustion control occur at cold-start and idle operation conditions [14], [15]. PCCI combustion refers to a type of combustion where very advanced start of injection of fuel strategy is applied in the compression stroke. Therefore, a partially homogeneous mixing of fuel vapor and air occurs prior to combustion. The resulting mixture has a homogeneity that is between conventional diesel and HCCI combustion. In the PCCI concept, injection and evaporation of the fuel happen before combustion, and multiple sequential auto-ignitions happen at various locations, which is controlled by chemical kinetics [16]. In PCCI combustion, a more uniform lean mixture is obtained due to longer ignition delay compared to CDC. This results in lower flame temperatures, which reduce the production of NO_x and soot emissions [17], [18].

The PCCI concept has benefits of ultra-low NO_x and soot emissions, as well as higher efficiency and versatility in using several types of fuels. However, there are also disadvantages associated with PCCI engines, including cylinder wall wetting, challenges in forming the fuel-air mixture, difficulties in controlling combustion timing, and a potential for high UHC and CO emissions.

1.2. Motivation of the Study

There are various proposed solutions to reduce problems related to combustion in heavy-duty CI engines in the previous section. These solutions include using multiple injection strategies, optimizing fuel rail pressure, reducing compression ratio, optimizing EGR rate, utilizing narrow spray inclusion angle injectors, controlling intake temperature, and optimizing intake valve closing timing. However, there is currently no widely used commercial application of PCCI combustion in the automotive industry, and further research and technology development are needed to apply this type of combustion. The motivation of the thesis is to set-up, analyze and optimize PCCI combustion in heavy-duty DI diesel engines by experiments and CFD simulations, and introduce effective methods for reducing NO_x and soot emissions that can be applied in commercial applications.

1.3. Thesis Objectives – Methodology

The main objective of the thesis is to study the PCCI combustion in a single-cylinder DI diesel research engine by experimental and computational methods. Fuel spray characteristics, mixture formation, auto-ignition, premixed flame propagation, and engine performance and emission characteristics are analyzed to gain a better understanding of PCCI combustion to develop strategies suitable for emissions reduction of a full HDDI diesel engine without adversely effecting engine performance or fuel efficiency in part load operation.

To understand and optimize the characteristics of PCCI combustion in the engine, following topics are performed.

- 1- Conduct experimental studies of PCCI combustion under part load operation of the single-cylinder research engine to determine its performance and emissions characteristics.
- 2- Analyze the effect of multiple injections on spray penetration, spray wall interactions and mixture uniformity to improve in-cylinder mixing process, avoid wetting of cylinder walls by sprays, and reduce engine-out NO_x and soot emissions without compromising fuel economy at part load engine operation.

- 3- Investigate the effect of EGR on mixture formation, spray wall interactions, engine-out emissions, and fuel economy to improve mixture uniformity, reduce wetting of cylinder walls by sprays and control the start of combustion.
- 4- Study the effects of start of injection timing(s) on in-cylinder mixture formation, interactions of fuel sprays with the piston bowl and cylinder walls, PCCI combustion, engine-out emissions and fuel economy by Computational Fluid Dynamics simulations of the reactive flow which enable visualization of the mixture formation and combustion processes in detail, yielding proposition of design alternatives to reduce wall wetting.
- 5- Evaluate the effectiveness of combined split injection strategy and EGR rate in the base and early intake valve closing events to improve in-cylinder mixture formation and combustion phasing.

In this thesis, experimental methods and CFD simulation techniques are implemented to analyze the spray and combustion phenomena in HDDI Diesel engines. The objective is to develop a successful strategy for PCCI combustion at part load operation. Measured time history of the in-cylinder pressure, calculated variables from in-cylinder pressure, and engine-out emissions test data are utilized to evaluate the PCCI combustion. Spray dynamics and interactions of the fuel sprays with the piston bowl and cylinder walls are visualized by postprocessing the Computational Fluid Dynamics (CFD) simulation results. The study investigates the fuel vapor air mixture formation process in multiple injection strategies for a variety of EGR rates and compression histories of Early Intake Valve Closing (EIVC). The methods are utilized to optimize the performance and emissions of a heavy-duty CI engine for PCCI combustion under different operating conditions.

1.4. Layout of the Study

First chapter introduces the compression ignition strategies of conventional and low-temperature combustion. The chapter covers the background and motivation of the thesis, outlines the main objectives, and describes the methodology used.

Second chapter reviews the literature on the diffusion controlled and low temperature combustion modes of compression ignition engines. The chapter also reviews the formation mechanisms of NO_x , soot, UHC, and CO emissions. The implementation of

EGR technology is explored as a means of reducing the main pollutant, NO_x , in both conventional and LTC modes.

Furthermore, injection related parameters, implementation of control factors, geometric modifications, and engine technologies to facilitate PCCI operation mode are discussed. Overall, this literature review provides a comprehensive understanding of the various combustion modes and emission formation mechanisms in compression ignition engines.

The third chapter focuses on the experimental study of PCCI combustion. Detailed description of the engine, experimental setup, and data acquisition system used in the investigation are described in this chapter. The engine layout, dynamometer, measurement devices, and operating conditions are explained. Direct measurements of in-cylinder pressure and engine-out emissions, and calculations of the heat release rate time history, combustion, heat transfer, closed-cycle efficiency, and center of combustion were conducted to optimize the engine performance and emissions. The effects of start of injection (SOI) timing in a single main injection strategy, considering the influence of EGR rate and fuel rail pressure on engine performance and engine-out exhaust emission trade-offs, were investigated. To better understand the challenges of PCCI combustion, Computational Fluid Dynamic simulations were conducted to examine the effect of spray-wall interaction on engine performance and emissions. Multiple injection strategies having selected injection parameters across a range of EGR rates were then explored to reduce spray wall impingement problem. A double injection strategy with no-EGR and heavy EGR settings was considered to identify the optimal engine operation for PCCI combustion in terms of performance and emissions.

In Chapter 4 of this thesis, the focus is on the computational aspects of PCCI combustion. Specifically, reactive CFD studies are conducted to gain insight on the spray dynamics, flame propagation, and emission formation in the combustion chamber. In chapter 4, reactive flow CFD simulations are performed to visualize and understand PCCI combustion inside the combustion chamber. The first section outlines the modeling techniques and approaches employed. Subsequently, the study validates both conventional diesel and PCCI combustion simulations by experimental data. Additionally, a SOI sweep is performed to gain insight into spray dynamics, flame propagation, and emissions formation inside the combustion chamber. A computational study analyzes the effect of spray inclusion angle on liquid fuel-wall

interaction, engine performance, and engine-out exhaust emissions. Lastly, the chapter examines the combined effect of split injection strategy and EIVC on PCCI combustion operation.

In the final chapter, conclusions of the experimental and computational studies are stated, optimized engine operating parameters for PCCI combustion at low load are given, and future work for further investigation and implementation of potential technologies related to PCCI combustion is proposed.



2. LITERATURE REVIEW

2.1. Motivation Conventional Diesel Combustion

Diesel engine was invented by Rudolf Diesel in 1892. The engine is a 4-stroke engine, and auto-ignition of the combustible diesel fuel vapor-air mixture occurs at the end of the compression stroke. In the last 25 years, improvements have been made to increase engine efficiency, durability, and power density. High pressure direct fuel injection, well-designed combustion chamber geometries, and turbo-charged inter-cooled engines are some of the main advancements. DI diesel engines have become popular for heavy duty vehicles due to their high thermal efficiency, durability, low-speed torque levels, and reliability compared to spark ignited (SI) engines. DI diesel engines are now used in 96.6% of the heavy-duty vehicles in the transportation sector [19]. However, diesel engines face two significant challenges of NO_x and soot production during combustion [20].

The current regulatory framework for diesel engines demands compliance with increasingly stringent emissions standards, such as the RDE and the Worldwide Harmonized Light Vehicles Test Cycle (WLTC) under the latest LLC conditions. To meet these requirements, novel combustion modes and regenerative ATS have been developed to effectively control emissions during realistic urban, rural, and motorway driving scenarios. Additionally, the testing protocol now includes cold-start, low load, and stop and go operations, further emphasizing the need for advanced emission-control technologies in diesel engines [6], [21].

In conventional DI compression ignition engine, highly pressurized fuel is injected into the engine combustion chamber in late stage of the compression stroke. The fuel then undergoes atomization, evaporation, and mixing with boosted air under high pressure and temperature of the combustion chamber, leading to auto-ignition. The combustion process that follows is diffusion-controlled and relies on the air-fuel mixing capabilities of the rich mixture.

Diesel combustion process develops in several steps as shown in **Figure 2.1**. After injecting the diesel fuel into the combustion chamber, fuel droplets start to evaporate,

and this can lead to a negative impact on Apparent Heat Release Rate (AHRR) curve. The duration between the start of injection and the start of combustion which is indicated by the initial increase of the AHRR curve is called the Ignition delay. During this period, fuel mixes with the air and then the mixture rapidly auto-ignites due to prevailing high pressure and temperature, causing a sudden increase in AHRR. This is the second step of diesel combustion that is called premixed combustion in fuel rich conditions. After premixed burn, AHRR drops back rapidly and then slowly rises to the second peak value. In this step, a diffusion-controlled combustion occurs. Combustion speed is controlled by the air-fuel mixing rate and the flame occurs under stoichiometric regions.

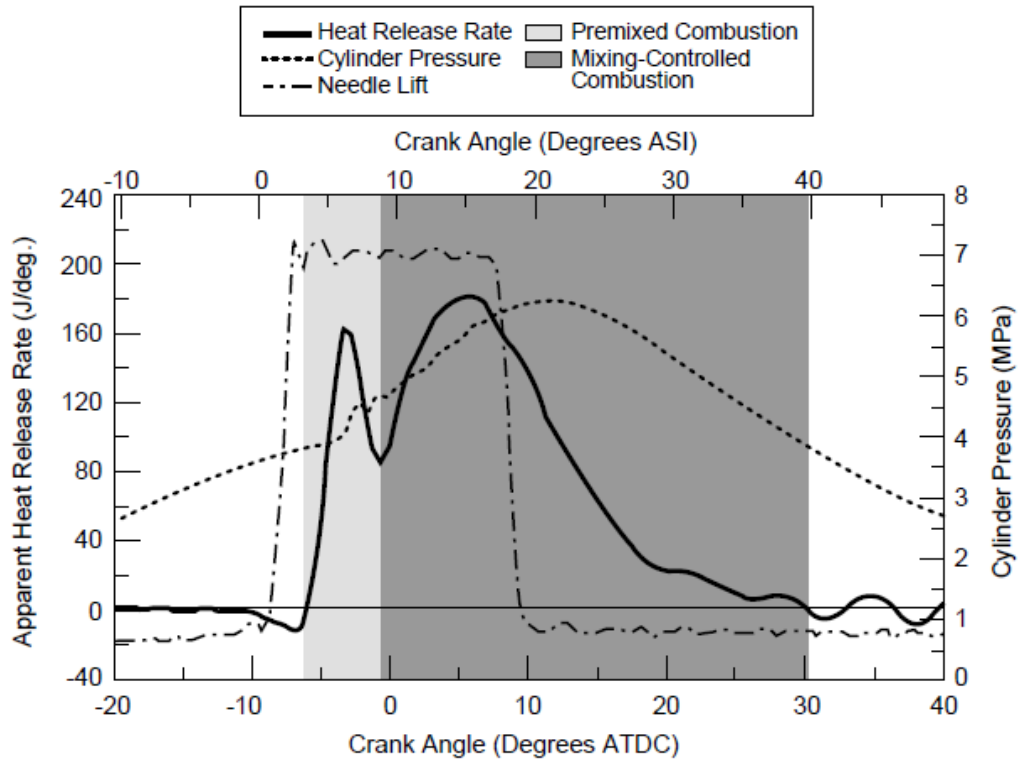


Figure 2.1: Example Apparent Heat Release Rate, In-cylinder Pressure, and Injector Needle Lift Profile for high fuel load operation [22].

Diffusion-controlled combustion process of diesel combustion, which is a complex phenomenon that involves several distinct regions, including the liquid fuel, air-fuel vapor mixture, fuel-rich premixed combustion, high temperature oxidation reaction, thermal NO_x production and soot formation and oxidation is described by Dec, who aims to provide a comprehensive understanding of the various intricacies associated

with the diffusion-controlled combustion process [22]. In **Figure 2.2**, the potential areas for soot creation and oxidation, and NO_x formation in the theoretical model of injection-controlled combustion are shown. Soot is formed in the downstream area of the premixed flame in the fuel rich region, while it is oxidized by hydroxyl radical (OH) generated in the diffusion flame, and oxygen can also be expected to oxidize soot particles outside of the region. NO_x formation happens in the outer region of the diffusion flame where the temperature is high and oxygen-rich conditions provide an ideal environment for NO_x to form.

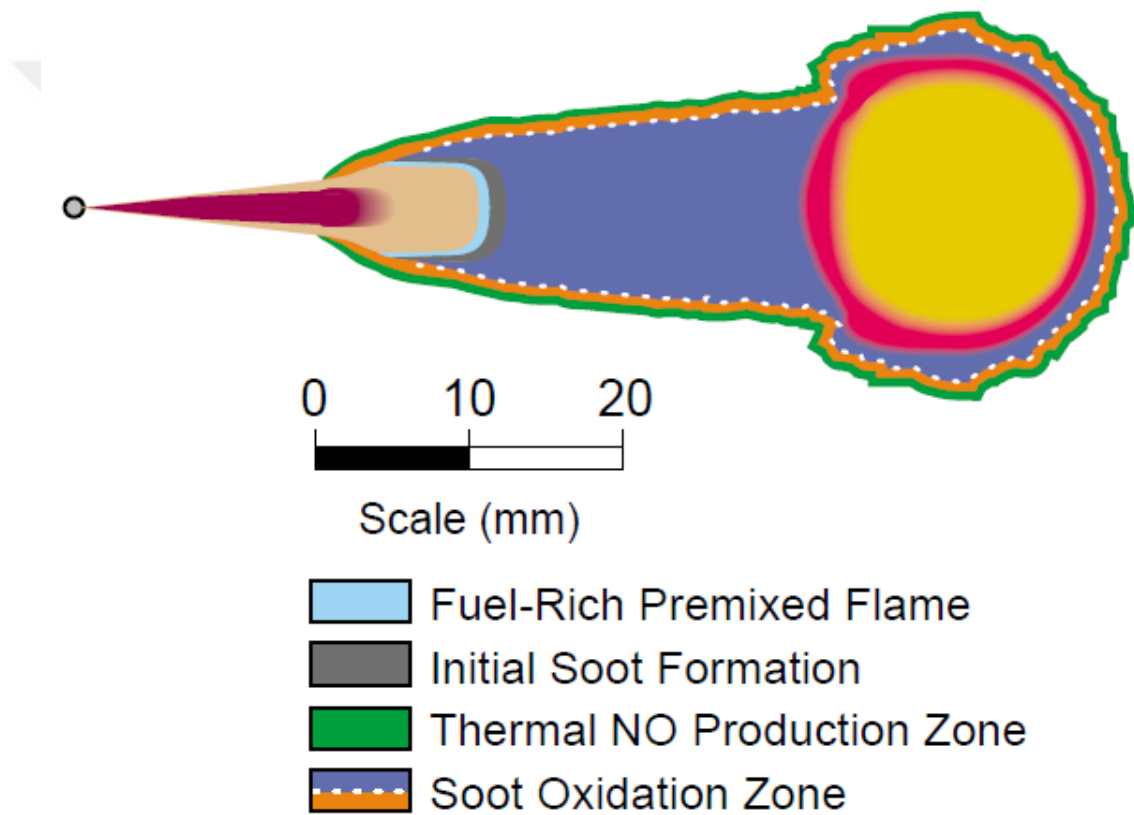


Figure 2.2: Dec's conceptual DI diesel combustion flame model during diffusion-controlled combustion [22]

Overall combustion process of typical DI CI engine can also be defined by heat release rate diagram. The heat release rate diagram provides valuable information about the combustion process, including the timing and rate of combustion, the peak pressure, and the heat transfer to the cylinder walls. These parameters are critical for understanding engine performance, emissions, and efficiency. By analyzing the heat

release rate diagram, engineers can optimize engine design and control strategies to achieve better fuel economy, lower emissions, and improved reliability. Therefore, the heat release rate diagram is an essential tool for studying and improving the combustion process in DI CI engines. The equation (2.1) considers the cylinder volume, the mass of air and fuel in the cylinder, and the energy released during combustion [23].

$$\frac{dQ_{net}}{dt} = \frac{dQ_{ch}}{dt} - \frac{dQ_{ht}}{dt} = \left(\frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} \right) \frac{d\theta}{dt} \quad (2.1)$$

where, Q_{ch} is the chemical heat released by combustion, Q_{ht} is the heat exchanged by the gas from cylinder walls during combustion, γ is the isentropic coefficient, p is the in-cylinder pressure, V is the volume of the combustion chamber, θ is the crank angle and t is the time.

2.2. Formation of Pollutants

2.2.1. Nitrous Oxides Formation

Internal combustion engines mainly produce mono-nitrogen oxide (NO) and Dinitrogen monoxide (N₂O) species, and the total amount of these species is called NO_x emissions. In diesel combustion processes that are mainly diffusion-controlled, 70-90% of NO_x emissions are NO emissions, depending on the operating conditions [24]. Gasoline engines generate higher levels of NO_x emissions compared to diesel engines, but these emissions can be effectively eliminated using 3-way catalysts under specific stoichiometric conditions [25]. On the other hand, diesel engines require ATS systems due to lean operation conditions. Latest (EU6) emission legislation requires a NO_x limit on a drive cycle with a peak limit. Proposed emission legislation also limits NO_x emissions, besides imposing a separate N₂O limit due to its higher greenhouse impact. There are three different mechanisms that form NO_x emissions: thermal, prompt, and fuel. The fuel-related NO_x mechanism is related to fuels that include N atoms; however fossil diesel fuels do not include any N atoms. The prompt NO formation process is not available in diffusion-controlled combustion because prompt NO reaction pathways require very low temperatures, near stoichiometric and rich flames, under the presence of hydrocarbon radicals.



In the reaction mechanism that is shown in **Figure 2.3**, hydrocarbon radicals in the presence of nitrogen are converted to hydrogen cyanide and molecular nitrogen. This unstable nitrogen can easily be converted to NO.

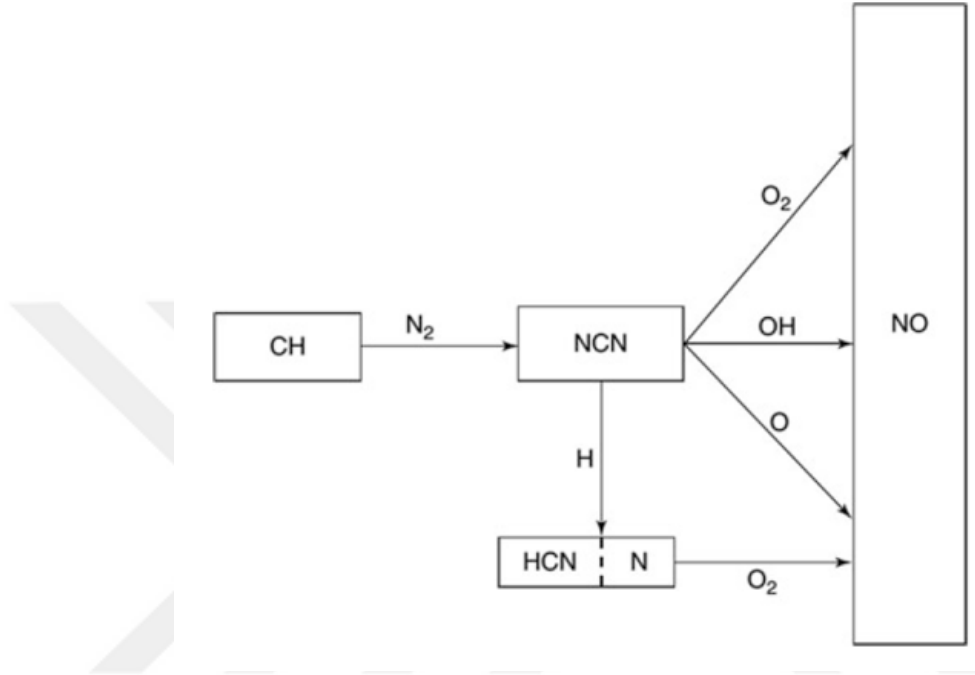


Figure 2.3: Prompt NO_x mechanism [26].

A significant portion of NO emissions is produced through the thermal NO mechanism, which occurs at temperatures above 1850K in the presence of disassociated oxygen atoms. In diesel spray combustion, the temperature ranges from 2500-3000K in the stoichiometric mixture zone. The Zeldovich model describes the thermal NO mechanism, which involves three reversible reactions known as the extended Zeldovich mechanism [27], [28].



The simplified model indicates that the maximum production rate of NO exhibits an exponential relationship with temperature in the presence of O₂ concentration [29].

$$\left[\frac{d(NO)}{dt} \right]_{max} = 1.70 \times 10^{17} T^{-\frac{1}{2}} \exp \left[\frac{69750}{T(K)} \right] x(O_2)_{eq}^{\frac{1}{2}} (N_2)_{eq} \frac{mol}{cm^3 s} \quad (2.6)$$

Diesel spray exhibits temperature levels ranging between 2500-3000K in the diffusion-controlled combustion zone. Optical investigation of NO formation confirmed that thermal NO is generated around the closed flame where high temperatures prevail due to stoichiometric combustion, in the presence of O₂ from the air [30].

In contrast, the reverse reaction of the first elementary reaction is impossible thermodynamically due to temperature decrease during the engine's expansion stroke, which effectively prevents reverse reaction of NO to N₂. The proportion of NO_x emissions formed by NO₂ is contingent upon the operational parameters of the engine, ranging from 10% to 30%. The production of NO₂ is described by the equation (2.7) [23].



Conversion of NO to NO₂ mechanism occurs at high temperature and presence of Oxygen. But the limited time and sudden expansion phase of the engine eliminates high production rate of NO₂. On the other hand, NO₂ is converted to NO on the reverse conversion where temperature levels and time is sufficient of the reaction in the expansion stroke of the engine. The reaction mechanism of NO₂ to NO is given by equation (2.8) [26].



2.2.2. Nitrous Soot Formation

Formation of soot in internal combustion engines is a complex process that involves several steps: Pyrolysis, nucleation, coalescence, surface growth, and agglomeration. During the pyrolysis process, fuel is thermally cracked into smaller molecules in oxidant lean environment and at elevated temperatures, such as poly-aromatic hydrocarbons (PAH) and acetylene (C₂H₂), which are the precursors for soot formation. In addition, cyclopropenium (C₃H₃) and benzene (C₆H₆) are also known as precursors in the soot formation mechanism [31].

As the research conducted by Tree and Svensson, the nucleation step involves the combination of these soot precursor molecules to form soot particles. In the subsequent surface growth step, the hydrocarbon mass around the soot molecules increases due to polymerization reaction. Finally, the soot particles combine to form large groups in the last process [18]. These steps are shown in **Figure 2.4**.

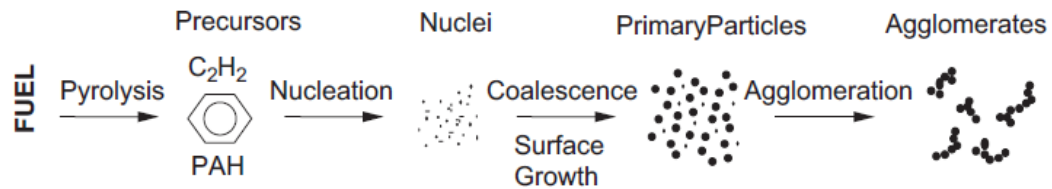


Figure 2.4: Soot formation process

In conventional diesel combustion, soot is generated in a region of locally higher concentration downstream of the spray on the premixed combustion event, where the temperature is rapidly increasing. However, it should be noted that most of the soot particulates generated during combustion are oxides, particularly in the later stages of the process. The rate of production and subsequent oxidation of soot throughout the expansion stroke is what ultimately determines the cumulative amount of engine-out soot emissions [32].

In the diffusion-controlled flame, soot is formed inside the diffusion flame where oxygen have consumed, and temperature levels are above 1700K up to 2200K [22]. Soot production is increasing during spray duration period due to oxygen lean region inside the flame. Subsequently, with the introduction of oxygen availability in the combustion products through the effects of diffusion and convection, soot amounts are decreasing. This is due to the dominant soot oxidation rate, which is aided by the high temperature. The process of soot oxidation is primarily facilitated by OH molecules, which are formed at high temperatures and in the presence of O_2 molecules [33], [34].

2.2.3. Unburned Hydrocarbon Formation

Hydrocarbon emissions refer to the release of various organic compounds, including pure hydrocarbons and fuel compounds, that occur due to incomplete combustion in areas of low oxygen concentration and temperature within the combustion chamber.

At least, a temperature level of 1200 K is required for UHC oxidation, which is valid for almost all types of hydrocarbons [35]. Remaining engine-out UHC and CO emissions are catalytically converted to CO₂ emissions in the DOC present in the exhaust ATS [36].

In conventional diesel engines, employing advanced diesel fuel injection causes a longer combustion delay, promoting greater uniformity in fuel-air mixing and resulting in a substantial reduction of UHC emissions. Conversely, incorporating EGR leads to an increase in UHC emissions due to the decreased oxygen concentration in the diluted intake charge, as well as a decrease in heat rejection and combustion temperature [37]. In the diesel engine exhaust, mono-aromatic hydrocarbons (MAH's) and PAHs are produced due to pyrolysis and inhomogeneities due to local/regional mixing characteristics and in-complete combustion [38].

In diesel combustion, almost all the fuel is combusted. However, incomplete combustion can be more prevalent in LTC modes. Because combustion takes place on very low temperature and very lean conditions. The primary cause of UHC production in diesel engines is the use of excessively rich or lean mixtures. The process of complete or incomplete combustion mechanisms are shown in **Figure 2.5** [39].

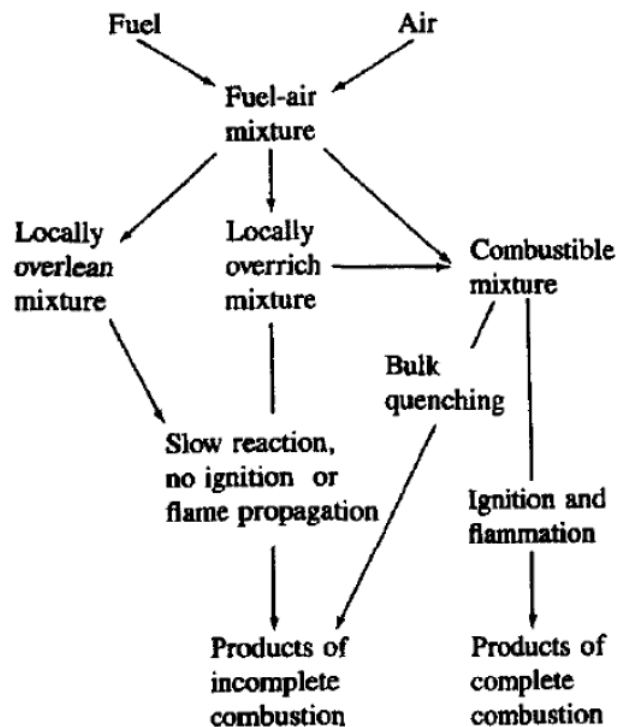


Figure 2.5: Characteristics of air-fuel mixture in the combustion.

In the phase of premixed delay of diesel combustion, in the downstream of the fuel jet, a fuel rich zone inside the flame core becomes a undermixed region where fuel is not totally oxidizes due to lower amount of oxygen, resulting in significant UHC production. Additionally, late-stage injection events can lead to reduced fuel atomization and lower air-to-fuel mixing capabilities due to decreased spray plume pressure and velocity. Because most injectors are in the center of the cylinder axis, this can further limit air mixing and velocity, additional UHC emission increase. The injector tip sac volume can also contribute to UHC emissions, as it contains a small amount of fuel that evaporates after the injector closes. Although reducing the injector tip sac volume is generally desirable, it can also help compensate for pressure oscillations and reduce soot emissions [40].

Over-mixing of fuel with oxygen is another potential cause of UHC emissions. When the fuel amount is over-mixed with oxygen outside of the diffusion flame, incomplete combustion can occur, resulting in unburned hydrocarbons. Although these fuels are typically burned during diffusion flame propagation, some may escape from high temperature zones, causing incomplete combustion.

Another mechanism that hydrocarbons are formed in engines is that flame quenches near the walls and crevice volume of the cylinder. When the engine is operating at low load, the flame propagation is limited and mostly localized within the piston bowl, but at high load, it spreads to the cylinder walls and is quenches due to cold temperature of the walls. This can happen when the fuel injection is too high or lasts too long, causing the fuel vapor or intermediate species that is not completely reduced. Low oxygen concentration and lower temperature can increase hydrocarbon production near cylinder walls. Additionally, if the swirl motion inside combustion chamber is not well-tuned with the number of injector nozzles, adjacent spray plumes can collide and create regions with low oxygen and high temperature, leading to excessive soot and UHC production [41].

Lubrication oil in an engine can contribute to the production of UHC inside the combustion chamber. A small amount of oil can get into the combustion chamber through the piston rings, where it can react as a fuel in the crevice volume, and it can be considered as a source of UHC production.

LTC regimes exhibit a phenomenon where the poor atomization of fuel leads to spray impingement, which, coupled with the low temperature in the combustion chamber, results in the production of UHC in the vicinity of the cylinder liner and piston bowl surfaces, as well as within the crevice volume. A more detailed analysis of these processes and their impact on UHC emissions in LTC engines are discussed in the following chapters.

2.2.4. Carbon Monoxide Formation

Carbon monoxide is produced through incomplete combustion in over-rich mixtures that have insufficient oxygen for complete oxidation of CO to CO₂. This occurs in the relatively low temperature environment of early or retarded combustion phasing [42].

As the fuel-to-air ratio moves from a rich condition to a stoichiometric or even leaner condition, there is a linear reduction in CO production. The reduction in CO production is attributed to the increase in oxygen availability and the more complete combustion of fuel molecules as the mixture becomes leaner [23].

In conventional diesel engines, excessive CO emissions is often observed in retarded combustion timings, which lead to a sudden decrease in temperature due to expansion cooling effect. Since, engines operating under conventional diesel or LTC conditions are always working under lean combustion, and CO emissions are produced under conditions of low temperature and lean combustion. It is worth noting that the reaction mechanism involved in the conversion of CO to CO₂ is highly sensitive to temperature, with the temperature range of 800-1400K gas temperatures are suitable CO formation [35]. In the proposed mechanisms, the fuel undergoes a series of chemical transformations, starting production of peroxides to aldehydes, and then to ketones and ultimately to carbon monoxide through subsequent reactions [40]. According to the provided reaction mechanism given by equation (2.9), the presence of oxygen in elevated temperature facilitates the oxidation of CO to CO₂.



OH radical is crucial in the reaction mechanism of CO to CO₂. OH radical is started to produce at temperatures above 1450-1500K during the combustion process, and its concentration exponentially increases with rising temperatures [43], [44].

Therefore, in conventional engines with optimized combustion timing can reduce CO emissions by operating high combustion temperature under lean engine operation. On the other hand, in LTC operation, due to lower combustion temperature values, CO emissions are increasing dramatically.

Use of DOC in ATS systems in commercial heavy-duty engines eliminates more than 99.9% of the CO and UHC emissions of engine out emission. It also mentions that the DOC needs to be heated to temperatures above 200-250°C for effective operation [45]. However, under heavy EGR rate operation, which can be used to control NO_x levels, can increase CO and HC production rates during LLC conditions when the DOC catalyst is below light off temperatures [46].

2.2.5. Nitrous Exhaust Gas Recirculation (EGR)

EGR is a very usable and common technology to reduce NO_x engine out emission in diesel vehicle engines. In the application, exhaust gas is transferred from exhaust manifold to the intake manifold through a pipeline. A controller valve is used to supply demanded EGR flow and in most applications, a water-cooled heat exchanger is used to cooled down exhaust gas temperature of the charge. The rate of EGR mass flow is calculated by considering the cylinder charge mass, fresh air mass flow, and volumetric efficiency of the engine, based on intake mass flow and pressure and temperature values.

The use of cooled-EGR is now mandatory in diesel passenger and commercial vehicles due to stricter emissions regulations and started to apply to SI gasoline engines to reduce knock intensity in high specific powered engine applications.

NO_x emissions are produced in high-temperature environment, that EGR slows down the heat release in the combustion chamber. The use of EGR employs three methods to decrease the peak heat release rate of combustion.

The implementation of EGR within the intake air system results in a diluted oxygen concentration within the intake charge. Consequently, the peak temperature of combustion is reduced, due to the reduced oxygen concentration in the combustion chamber. The attenuation of oxygen concentration within the combustion chamber leads reduction in the ignition delay of the premixed burn, resulting in a lowered peak heat release rate [47].

Secondly, a decrease in the amount of oxygen present results in less oxygen being available in the area surrounding the flame. As a result, the homogeneity of the mixture of air and fuel is compromised. This can lead to an increase in combustion duration and a decrease in the peak heat released during the process. This reduction in heat release rate can also lower the production of NO_x [48].

Thirdly, the presence of CO_2 and water (H_2O) in the EGR, has been found to have a significant impact on the combustion process. This is due to the endothermic dissociation reaction of these species, which causes the combustion to slow down. As a result, the concentration of NO_x in the exhaust gas is reduced, primarily due to the chemical effects of EGR [40].

In addition, the presence of CO_2 and H_2O in EGR can also increase the specific heat capacity of the engine's intake charge, leading to lower peak temperatures during ignition and combustion. However, the thermal effect of EGR is limited comparing the chemical effects [49]. The use of EGR causes the ignition timings to be delayed in all types of engines, including both CI and SI engines, and in both conventional combustion and HCCI and PCCI combustion modes [17], [29].

2.3. Low Temperature Combustion (LTC) Regimes

In LTC strategies, the aim is to separate injection and ignition as much as possible. In contrast to conventional diesel engines, where the ignition delay is always negative, LTC engines have a longer ignition delay than injection period, resulting in a positive ignition dwell. This positive dwell time enables a better fuel-air mixing and the development of a lean, and homogeneous mixture, ultimately results to low temperature combustion [50]. The progress of the combustion can be shown in Equivalence Ratio – Temperature map. Formation of soot, NO_x and even UHC emission zones can be illustrated for investigating the conventional diesel and LTC combustion regimes.

In the beginning, the Equivalence Ratio-Temperature maps were created through experiments using combustion bombs and laser extinction techniques to measure soot, NO_x , and UHC emissions [51]. Alternatively, these maps can also be produced through simulations using kinetic reaction models, which are specific to a particular fuel type and pressure, as shown in **Figure 2.6** [52].

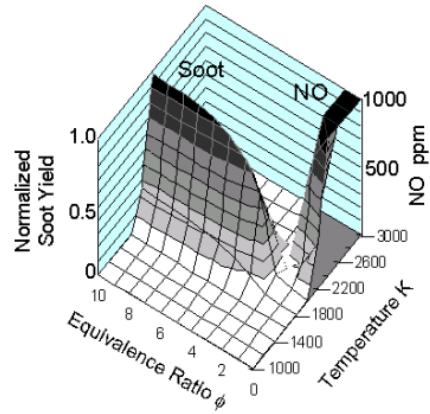


Figure 2.6: Calculated Equivalence Ratio – Temperature map.

It has been observed that soot is generated at temperatures ranging from 1700-2500K when the equivalence ratio exceeds 2, while NO_x is produced when the temperature is above 2200K, but the equivalence ratio is below 2. In the traditional diesel process, the combustion process begins at a high equivalence ratio and low temperature. As the temperature rises, most of the combustion area enters the soot production zone, where the fuel-rich mixture prevails. Once the fuel is consumed, the temperature continues to rise, and the combustion zone transitions into the NO_x production zone, where the equivalence ratio drops below 2.

To eliminate the production of soot and NO_x , combustion should occur in low temperature and a lean ratio of air to fuel conditions. The regions of alternative low temperature combustion modes are visually demonstrated in **Figure 2.7**.

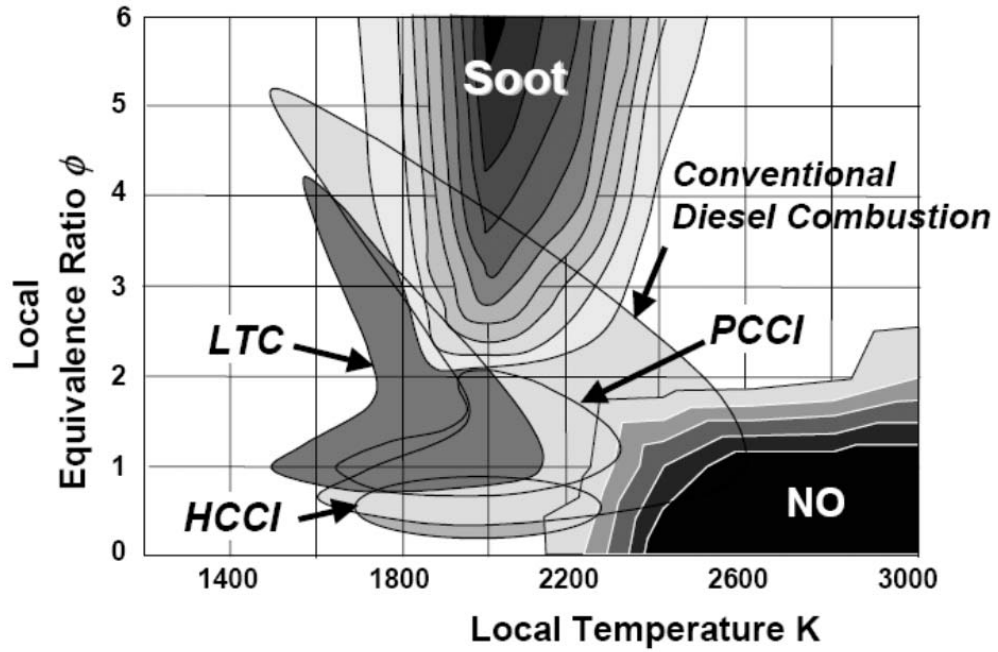


Figure 2.7: LTC and PCCI concept on Equivalence Ratio - T map [53].

Typical injection timings to perform LTC concept is defined in shown in **Figure 2.8**. HCCI, PCCI, and modulated kinetics (MK) all manipulate injection timings to improve pre-ignition mixing. By injecting fuel into a cooler environment, ignition is delayed, allowing for a greater opportunity for fuel and air to mix. HCCI and PCCI employ early injection timings, while MK utilizes late injection at or after top dead center (TDC).

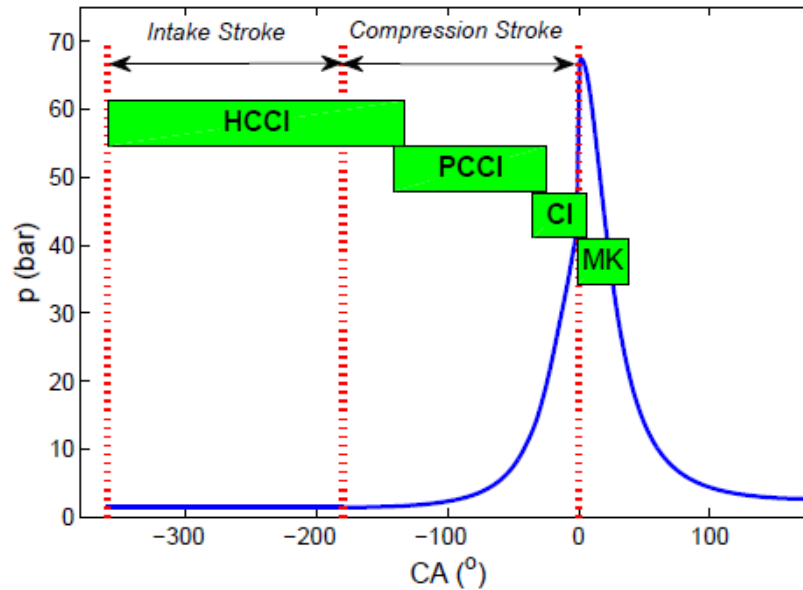


Figure 2.8: Typical injection timings for different combustion modes.

2.3.1. Homogeneous Charged Compression Ignition (HCCI) Combustion

HCCI combustion has shown great potential in achieving ultra-low emissions of both NO_x and soot, thanks to its unique combustion process that combines the advantages of both spark ignition and compression ignition [54].

In HCCI combustion strategy, the use of very advanced injection timings is used to ensure a homogenous mixture of fuel and air. This mixture preparation is achieved through either port fuel injection or very early direct injection. Unlike in spark ignited engines where combustion is initiated by a spark, in HCCI engines, the homogeneous charge is self-ignited and combustion phasing is primarily controlled by chemical kinetics. Combustion occurs simultaneously in various locations once the auto-ignition temperature is reached. Unlike in spark ignited premixed charge engines, where combustion is initiated by a spark, in HCCI engines, self-ignition is triggered by the pressure and temperature during the compression stroke, dominated by chemical kinetics [55].

The HCCI concept operates on the principle of simultaneous ignition of multiple locations, resulting in rapid combustion without flame propagation. Fuel is consumed gradually on several reaction zones locally, leading to an increase in in-cylinder gas

temperature due to exothermic reactions. Compared to conventional diesel combustion, HCCI combustion occurs in a short duration and generates a significantly higher heat release rate [29]. In HCCI, combustion is decoupled from injection timing, and a prolonged ignition delay required [56].

Lean and homogenous mixture formation in HCCI combustion results near-zero NO_x production due to lower combustion temperatures. Additionally, lean engine operation, characterized by a local equivalence ratio ($\phi < 2$) effectively eliminates the formation of soot [57]. Furthermore, a lean fuel-air mixture is utilized to regulate the rate of heat release, thereby effectively controlling the temperature of combustion.

There are several drawbacks of HCCI combustion in operation. One of these drawbacks is that low volatility fuels like diesel are difficult to use because they do not vaporize easily and can cause spray wall impingements [58]. Diesel fuel cannot evaporate easily on low temperature environment of early direct or port injection [59].

The phenomenon of wall impingement has been found to result in a rich combustion process within the crevice volume, leading to an increase in emissions of CO and UHC, as well as oil dilution [60]. Long separation of combustion phasing and injection requirement of HCCI combustion is not viable for diesel fuel due to its low self-ignition temperature. However, despite this limitation, there are some HCCI engine applications that have already been implemented in commercial settings for SI gasoline engines [61].

Combustion phasing and control presents a challenge in the HCCI process. The self-ignition characteristics of HCCI combustion is influenced by various factors such as intake charge temperature, cylinder wall temperature, EGR rate, compression ratio, engine load, fuel injection amount, and the residual gas from the previous cycle. Maintaining a stable combustion is particularly difficult as it can result in misfire at low loads and knock at high loads [62]. The occurrence of misfire in combustion due to a low load and low temperature environment can be eliminated by the implementation of boost temperature control and spark-assisted combustion techniques [63], [64].

To be able a high load operation of HCCI combustion, heavy EGR usage and reduction of effective compression ratio (CR) by using advanced early/late intake valve timing strategies are proposed [54], [65], [66], [67].

Furthermore, HCCI has the disadvantage of producing higher levels of UHC and CO emissions compared to diesel combustion. Low temperature combustion and over-lean zones are results excessive UHC and CO generation and combustion is not totally completed [68].

In addition, flame can be quenches closed to the cylinder walls and in the crevice region, leading to the production of UHC and CO emissions [69], [70].

2.3.2. RCCI Combustion

High octane, low reactivity fuel is injected directly into the cylinder in very early in the compression stroke or fuel is injected into the ports during intake event. Additionally, the high volatility properties of the low reactivity fuel facilitate the mixing of fuel and air, ensuring efficient combustion. Then, high reactivity fuel is injected in compression stroke directly into the combustion chamber to start auto-ignition. Overall, RCCI combustion represents a promising approach to improving the efficiency and reducing emissions of internal combustion engines [71]. The idea is to control the phasing and duration of the combustion process in an engine by using two different reactivity of fuels. This involves using multiple injection methods and adjusting EGR rate to improve efficiency and obtain ultra-low NO_x and soot emissions [29]. SOI of the high reactivity fuel plays a crucial role in determining the energy release during the combustion process. Advanced injection timing of high reactivity fuel, which is known as overmixing, can result in short ignition delays and consequently, leads to shorter combustion durations. Conversely, late injection of high reactivity fuel, which is called undermixing, leads to long ignition delays and can result in longer combustion durations [72].

RCCI combustion of natural gas/diesel or gasoline/diesel fuels are investigated in the literature. Natural gas/diesel RCCI combustion has been shown to provide significant reductions in NO_x emissions while maintaining high engine efficiency [73]. The addition of natural gas also improves the combustion stability and reduces the rate of heat release, resulting in lower engine noise and vibration [74]. Similarly, gasoline/diesel RCCI combustion has also been shown to provide significant improvements in engine efficiency and emissions. Gasoline has a higher reactivity than diesel, which allows for better mixing of the fuels and a more complete combustion process. This results in reduced emissions of PM and NO_x. Gasoline/diesel RCCI

combustion also provides a wider operating range and improved combustion stability compared to HCCI combustion [75], [76], [77].

The primary drawback of HCCI combustion lies in the challenge of determining optimal fuel's reactivity for controlling the combustion process. Requirement of two types of fuels with different levels of reactivity makes the engine design complicated and requires separate two fuel system, which can be expensive and inconvenient for drivers. To solve this problem, researchers are looking for a single fuel that can work for both types of combustion by adjusting the fuel cetane number [78].

On the other hand, using a combination of high reactivity biodiesel and low reactivity ethanol can be an effective way to achieve a fuel source that is free of fossil fuels. It is likely being made in the context of a larger academic and environmental discussion about alternative fossil free fuel sources and their potential benefits and drawbacks [79]. Overall, the literature indicates that RCCI combustion can offer substantial benefits in terms of improving engine efficiency and minimizing emissions. Nevertheless, there is a need for further investigation to refine the combustion process, address the dual fuel system requirement, and enhance the durability of the engine components.

2.3.3. PCCI Combustion

PCCI is a combustion mode between HCCI and CI combustion modes. The aim of PCCI combustion is to take advantage of the low levels of nitrogen oxides and soot produced by the HCCI advanced combustion mode in diesel engines, while also increasing efficiency. The idea is to realize a fuel mixture that is partially or fully premixed with air, and obtain a homogeneous mixture the engine, to prevent high levels of NO_x and soot emissions where combustion temperatures are lower than those typical of traditional diesel engines. The use of PCCI in conventional diesel engines is a promising approach to achieve improved fuel efficiency and reduced emissions. However, the use of diesel fuel in PCCI operation poses certain challenges due to its low volatility. Injecting diesel fuel into the intake ports can lead to issues such as excessive soot and hydrocarbon buildup, thereby effecting engine performance and emissions. Therefore, direct injection of diesel fuel is the preferred approach for PCCI operation [58]. In PCCI combustion, fuel is injected very advanced in the compression stroke. Injection and ignition processes are decoupled as in HCCI mode. Due to the

advanced injection timing, which causes low temperature and pressure levels inside the cylinder, there is enough time for fuel spray penetration and fuel-air mixing to achieve a uniform charge homogeneity prior to ignition in PCCI combustion [80]. In PCCI mode, combustion phasing control is possible by optimizing start of injection timing, number of injections, injection pressure and EGR level. On advanced injection timings, a fully PCCI mode can be achieved, while closed-to-TDC injections can result in partially premixed charged compression ignition that is like conventional diesel combustion. Using multiple injection strategies in PCCI combustion can improve fuel atomization, eliminate spray wall interaction, and results a better homogeneous fuel air mixing performance [81], [82], [83], [84].

Low temperature PCCI combustion is differ from mixing-controlled combustion. Liquid fuel penetration is much longer than conventional diesel combustion which is a potential source of UHC emission due to spray wall wetting. An updated conceptual model proposed to explain PCCI combustion shown in **Figure 2.9**. Combustion takes place in two ignition stages. In the first stage, energy released by the fuel ignition promotes the fuel evaporation. In the second stage, combustion takes place in well-mixed environment that, very low soot is formed. In the downstream of the second stage, fuel-rich head vortex promotes soot production.

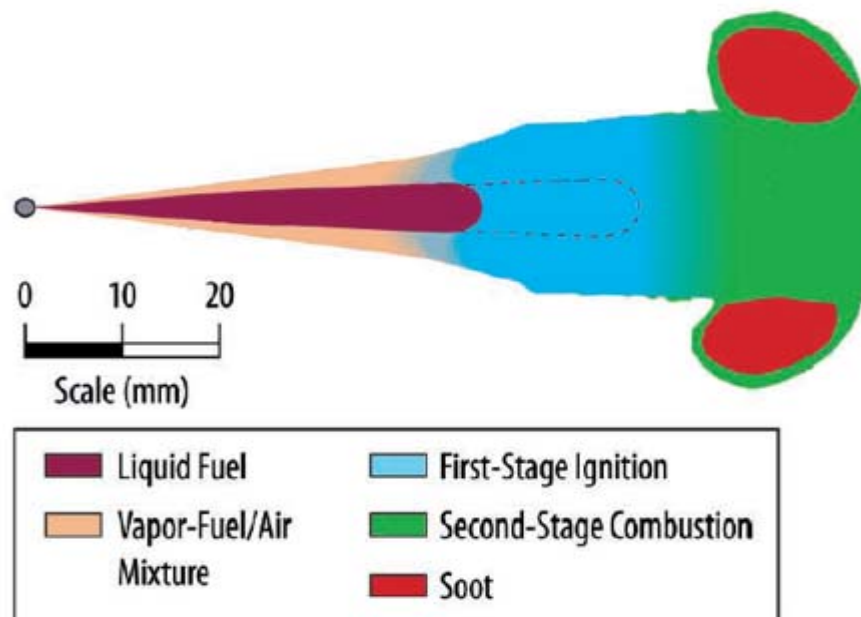


Figure 2.9: A concept model for advanced injection of PCCI Combustion [50].

The MK concept has been suggested to obtain ultra-low NO_x and soot emissions. It involves injecting fuel at the beginning of the expansion stroke, while concurrently implementing heavy EGR, increased injection pressure, and a high swirl rate to achieve a positive dwell. This approach results in lower combustion temperatures due to the EGR level and temperature reduction arising due to expansion of the combustion chamber, leading to reduced NO_x and soot emissions [85], [86]. But MK concept is not practical due to various factors. These factors include high swirl, EGR rate, and reduced compression ratio requirements that can reduce heavy-duty engine's volumetric and thermal efficiency, respectively. In simpler terms, the combustion concept may not be feasible due to its impact on the engine's efficiency and performance.

The UNIFORM BULKY Combustion System (UNIBUS) offers an alternative approach to minimizing NO_x emissions. This method employs advanced fuel injection and a main injection occurring after top dead center (ATDC) in the cool flame zone created by the initial advanced injection. It is crucial to optimize the main injection timing and temperature of the charge to avoid a diffusion-controlled flame and to minimize spray-wall interaction by optimizing the quantity of the first injection [87], [88].

Various injection strategies have been proposed including MULTIPLE stage Diesel Combustion (MULDIC), Homogenous charge intelligent Multiple Injection Combustion System (HiMICS), PREmixed Diesel Combustion (PREDIC) to extend load range, eliminate wall impingement risks, and lower the emission of UHC and CO associated with PCCI combustion [89], [90], [91].

Low volatility and high cetane number of diesel fuel poses challenges for mixture formation and combustion phasing control. To solve this issue, multiple injection strategies can be employed, adjusting the quantity of pilot and main injections, the use of EGR, and optimization of fuel pressure. These strategies enable the control of the local air-fuel ratio, combustion phasing, heat release rate, and temperature level of the combustion chamber. As a result, a LTC can be achieved, effectively eliminating NO_x and soot formation of high-temperature combustion modes [92], [93].

The achievement of a fully PCCI combustion can be applicable by using moderate to high EGR rates in conjunction with fuel injection timing. This approach can effectively decrease chemical reactivity and prolong ignition delay, enabling positive dwell time

and have a high degree of premixing of the charge. As a result, combustion temperatures can be lowered, early ignition can be avoided, and knock can be prevented [40], [94].

One method of controlling combustion phasing in diesel engines is through geometric and operational modifications on the engine that enable PCCI combustion. Lowering the compression ratio and applying an early or late intake valve closing the timing to reduce the effective compression ratio results a reduction on gas temperature of the fuel mixture during the compression stroke to achieve a great control over the timing of combustion in PCCI engines [95], [96], [97].

On the other hand, UHC and CO emissions are the products of PCCI combustion because of LTC characteristics [25]. As the EGR level is increased, there is a noticeable reduction in the temperature of combustion and delay in the start of ignition can also have a negative impact on the oxidation rate of soot, UHC and CO, particularly in areas where the oxygen concentration is lower due to the presence of EGR [98].

One of the limiting factors of PCCI combustion is, steep pressure rise rate of LTC combustion leads combustion noise in the engine at high load operating conditions [99], [100].

When using PCCI combustion at moderate engine loads, there is a problem with the fuel spray interacting with the cylinder walls. This is because the advanced injection timing, which means the temperature and pressure in the cylinder are lower, limiting spray atomization and evaporation. This will result excessive UHC and CO emissions, especially in the crevice volume. To solve this problem, a narrow cone spray angle can be used to eliminate the spray wall interaction [101]. In addition, Lee and Kim studied a dual injection with a narrow cone injector of 60°. They optimized the first advanced injection with a late second injection in the compression stroke to reduce NO_x and CO emissions while maintaining high combustion efficiency [102]. On the other hand, using a narrow cone injector will bring some risk on fuel-air mixing in high load conditions [25], [103]. Closed multiple advanced injection strategies of PCCI combustion can achieve a better homogenization of fuel air mixture that results slower heat release rate, very low NO_x emissions while maintaining relatively lower CO and HC emissions [104].

A dual row configuration of 15-hole injectors with a narrow spray angle is being suggested to avoid fuel impingement on the cylinder walls and improve the mixing of fuel and air in the piston bowl [105]. Use of hot EGR usage on very advanced injection of PCCI combustion can be effective strategy to reduce the spray wall impingement risk. In addition, increasing both charge and fuel temperature has shown to have benefits in reducing UHC emissions [106].

As a result of its unique characteristics, such as the ability to operate in extreme lean conditions and the ease of controlling combustion phasing by using multiple injections, optimized injection timing, and injection pressure levels, single fuel usage, PCCI combustion has clear advantages in heavy duty diesel engines under low load operation.

3. EXPERIMENTAL STUDY OF PCCI COMBUSTION

3.1. Introduction

The experimental studies conducted in this section are aimed at exploring the impact of various factors on both conventional diesel and PCCI combustion in Single Cylinder Research Engine. These factors include injection advance, multiple injection strategies, and EGR. The engine operating condition chosen for the study is the most commonly driven engine operation and is deemed suitable for engine operation. The objective of these studies is to gain a deeper understanding of how these factors influence combustion and to identify the optimal settings that can be used to improve engine performance. The research methodology involves carrying out a series of controlled experiments in a laboratory setting, using advanced measurement and analysis tools to collect and analyze data. The results of these studies are expected to understand the PCCI combustion and optimize the parameters to achieve low NO_x and fuel-efficient engine.

3.2. Single Cylinder Research Engine

The experimental studies were carried out on single-cylinder research engine. The aim of the engine is to perform combustion development activities serial production engine. The development target engine is Ford Otosan 13L ECOTORQ Heavy Duty Direct Injection (HDDI) engine which is currently used in Ford FMAX Trucks. The engine is a four-stroke, water-cooled, diesel fueled, heavy duty diesel engine with a 2.13 L displacement shown in **Figure 3.1**.

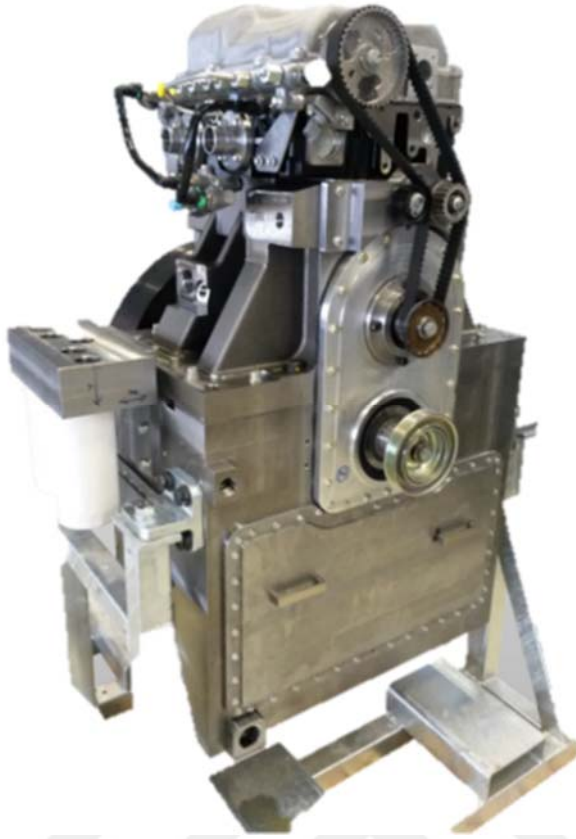


Figure 3.1: Single-cylinder HDDI research engine.

The combustion chamber and engine head geometry have been kept consistent with that of a multi-cylinder engine to ensure accurate representation of a production engine. The original injectors and piston are used same as the multi-cylinder engine. The engine has been equipped with a common rail fuel system capable of delivering up to 2500 bar pressure, based on the ECOTORQ 13L engine. Technical specifications of the engine and injector system are listed in **Table 3.1**.

Table 3.1: Technical specifications of Single Cylinder Research Engine.

Bore × stroke [mm]	130 × 160
CR	17.0:1
Swept volume [L]	2.1
Nozzle diameter [mm]	0.18
Number of injector nozzles	8
Spray Inclusion Angle [°]	146
Maximum injection pressure [bar]	2500
Intake valve opening [°CA Before TDC]	4
Intake Valve Closing [°CA After BDC*]	13
Exhaust valve opening [°CA Before BDC*]	40
Exhaust valve closing [°CA After TDC]	4

*Bottom Dead Center (BDC)

3.3. Experimental Setup

The AVL AC dynamometer is used to control the engine speed and regulate the demanded torque. It is connected to the engine with a driveshaft. The study measures the engine's performance in steady-state conditions at constant speed.

The dynamometer's automation system is responsible to maintain a constant crankshaft rotational speed, while the AVL Puma Open 1.4.2 automation system manages critical operational variables such as intake and exhaust manifold pressures, EGR rate, intake manifold temperature, and engine oil and coolant temperatures.

To determine the relevant parameters, AVL GU22CK pressure transducers are used to measure in-cylinder pressure values. Intake and exhaust pressure values are also measured with transducers to run the engine under fixed operation conditions, while k-type thermocouples are employed to monitor temperature values. The EGR flowrate and temperature are controlled using an EGR valve and EGR cooler.

Engine's intake air is sourced from the factory shop air and can supply at a pressure of up to 6 bar. To eliminate any potential variations of humidity in the supplied air, the intake air is chilled to 5°C, which results a constant humidity in the air. The boost pressure and temperature are regulated by the boost conditioner system, while a high-pressure external, cooled-EGR system is incorporated into the system. Additionally, an exhaust back-pressure valve is used to maintain the desired EGR flow and simulate the exhaust manifold pressure upstream of the turbine. The intake temperature is controlled by a water-heated air and water-cooled EGR system, which is integrated

into the boost conditioner system. The schematic diagram of the engine test bench setup is shown in **Figure 3.2**.

A vortex type flowmeter is used to measure the intake airflow and EGR flow in a test setup. Additionally, the EGR rate is calculated through volumetric efficiency calculation or by using the ratio of intake and exhaust manifold NO_x measurements. These techniques provide accurate and reliable data for evaluation.

EGR rate is determined through NO_x measurements by equation (3.1).

$$EGR_{rate} = \frac{[NO_x]_{intake}}{[NO_x]_{exh.}} \quad (3.1)$$

EGR rate can also be calculated based on volumetric efficiency shown in equation (3.2)

$$EGR_{rate} = 1 - \frac{\dot{m}_{airflow} RT}{\eta_V PV} \quad (3.2)$$

where, $\dot{m}_{airflow}$ is the intake air flow, R is the ideal gas constant, T is the intake gas temperature, η_V is the volumetric efficiency, P is the intake manifold pressure, V is the stroke volume.

To prevent any fluctuations in pressure, surge tanks with a capacity of approximately 200 liters are implemented in both the intake and exhaust manifolds.

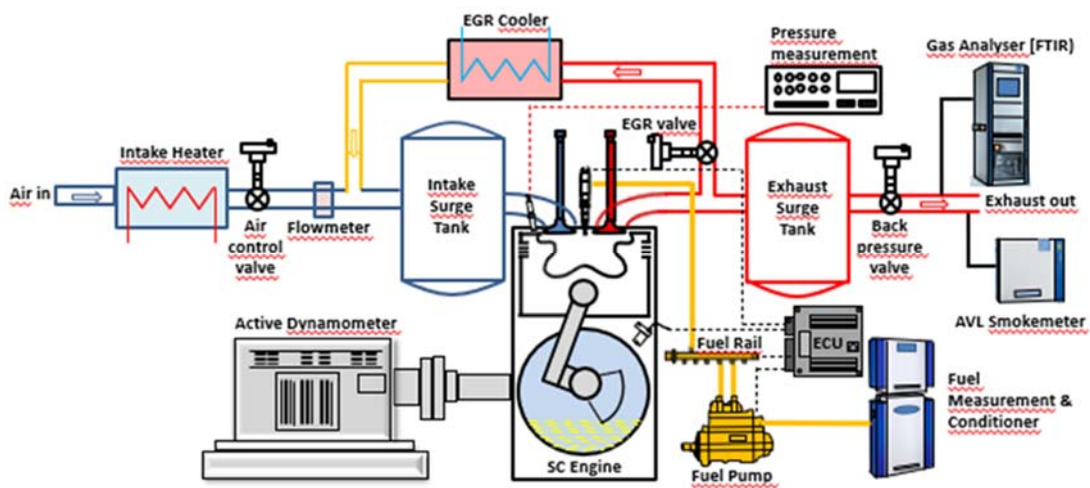


Figure 3.2: The schematic diagram of the engine test bench setup.

The control of fuel rail pressure, fuel injection timing, and amount of fuel injected is managed by a modified engine control unit (Bosch EDC17) of a multi-cylinder engine. The injector signals are monitored using a clamp ammeter, and the cylinder's crank-angle position is determined using a AVL 366C Angle Encoder.

In this study, an AVL IndiCom device is used to record the in-cylinder pressure measured by a piezoelectric pressure transducer (AVL GU22CK) with a sampling rate of 0.1°CA for one hundred cycles in an internal combustion engine. The recorded data was then processed to analyze various engine parameters such as in-cylinder pressure and heat release rate histories, indicated mean effective pressure (IMEP), crank angle at 50% mass fraction burned (MFB50%), ignition delay, combustion efficiency (CE), and indicated efficiency (η_i) based on different injection strategies and timings. Engine speed and torque in both motoring and braking conditions were controlled by the AVL Dyno-Road AC-Dynamometer. To measure the fuel flow rate, AVL 735S is used and conditioned it with AVL753C devices. NO_x, CO, and UHC emissions are measured by using a Fourier Transform Infrared Spectroscopy (FTIR) emission analyzer AVL SESAM i60 FT, and filtered smoke number (FSN) by using AVL 415 Smoke Meter. The specifications of these devices are listed in **Table 3.2**.

Table 3.2: Measurement device specifications

Measured Gas	Units	Range	Linearity	Reproducibility
CO	ppm	0–2000	<2.0% of measured value	<0.5 of range full scale
NO _x	ppm	0–1000	<2.0% of measured value	<0.5 of range full scale
Soot	FSN	0–10	-	+/-0.005 +6% measured value

The soot concentration of FSN can be calculated from the empirical correlation equation (3.3) [107].

$$Soot \left[\frac{g}{kWh} \right] = \frac{1}{0.405} * 4.95 * FSN * e^{(0.38 * FSN)} * \frac{(\dot{m}_{exhaust})}{\rho_{exhaust} * P_{engine}} \quad (3.3)$$

where, $\dot{m}_{exhaust}$ is the engine exhaust mass flow, $\rho_{exhaust}$ is the exhaust gas density, P_{engine} is the power of the engine.

The schematic diagram of the engine test bench setup is illustrated in **Figure 3.2**.

A standard of a EN590 fuel is used in the measurements. Properties of fuel in used in the measurements in shown in **Table 3.3**.

Table 3.3: Diesel fuel properties.

Density [kg/m ³]	830.1
Lower Calorific Value [kJ/kg]	42980
Cetane Number	55.5
Sulphur content [ppm]	<5
Viscosity@40°C [mm ² /s]	3215
Boiling point [°C]	160-360

3.4. Experiments of PCCI Combustion Strategies

Combustion process of PCCI is being studied with different levels of EGR up to 35% rates and fuel rail pressure of 800 bar. The study also includes the use of Double Injection Strategy (DIS) and Single Main Injection Strategy (SMIS) for engine operation. The parameters being varied in these different strategies include SOI, Single Pilot Injection (SPI), and Single Main Injection (SMI). The study considers exhaust temperatures below 220 °C where the engine operation point is selected at a Brake Mean Effective Pressure (BMEP) of approximately 3 bars, which is a just under the critical temperature range for efficient NO_x reduction using SCR. Operating conditions of the test engine is shown in in **Table 3.4**.

Table 3.4: Engine operating conditions.

Engine speed [rpm]	1100
Engine oil and coolant inlet temperature [°C]	80
Fuel and air intake temperature [°C]	25
Intake manifold pressure [mbar-abs.]	1425
Injected fuel mass [mg/stroke]	39
Fuel injection pressure [bar]	800
Air to fuel ratio (AFR) [kg air/kg fuel]	43-71:1 (Depending on EGR rate)

3.4.1. Single Main Injection Strategy (SMIS)

In this study, the effect of SOI ranging between -70 and 0 °CA ATDC on the combustion characteristics of single main injection strategy of PCCI combustion at 800 bar rail pressure, air to fuel ratio of 71:1 under no-EGR conditions are investigated in terms In-cylinder pressure and heat release rate (HRR) histories along with reference Diesel case. **Figure 3.3**, show that in the baseline Diesel case, where EGR rate is 7.1%, Pilot injection starts at -23 °CA ATDC with start of ignition (SOIgn) at -15 °CA ATDC, followed by SMI at -10 °CA ATDC, resulting in Diffusion-Controlled Combustion (DCC) that starts at -3 °CA ATDC. SOI timings between -25 and 0 °CA ATDC lead to diffusion-controlled combustion, with an ignition delay (ID) change between 7.5 and 10 °CA. In contrast, for Advanced Start of Injection (ASI), where injection starts between -50 ° and -30 °CA ATDC, partially premixed low-temperature combustion with SOIgn between -25 ° and -18 °CA leads to single-stage HRRs with peaks up to 275 J/°CA. SOI timings between -60 ° and -70 °CA ATDC result in wall wetting due to longer spray penetration and smaller HRR at relatively lower temperature and pressure environment. The effect of wall wetting in very advanced injection is evaluated in the simulation section of the study.

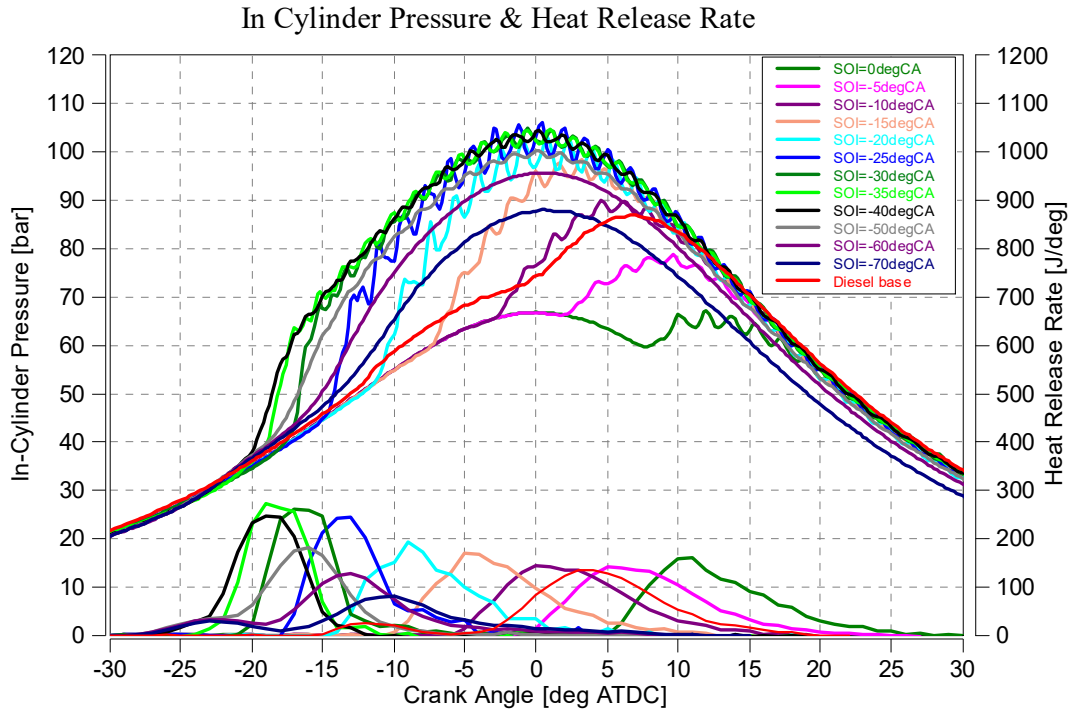


Figure 3.3: ICP and HRR histories according to °CA ATDC for various SOI timings in SMIS with no-EGR.

3.4.2. Effects of EGR Rate on PCCI Combustion for SMIS

In this section, impact of EGR on the in-cylinder pressure (ICP) and HRR histories of PCCI and diffusion-controlled combustion modes in a heavy-duty diesel engine are investigated. The experimental results are presented in **Figure 3.4** and **Figure 3.5**, which show the ICP and HRR histories plotted against crank angle (CA) for various SOI timings in the SMIS and reference CDC case (red) at 800 bar fuel rail pressure (FRP), with 18% and 35% EGR rates.

For PCCI operation with 18% and 35% EGR rates, the peak ICP decreases by up to 2.18 bars, while the midpoint of fuel burn (MFB50%) is delayed by up to 0.8°CA, and the peak HRR decreases by up to 7.18% (13 J/°CA) (at SOI of -50, -70, and -50°CA ATDC, respectively) compared to non-EGR cases. Conversely, for diffusion-controlled combustion, the peak ICP decreases by up to 3.6 bars, while MFB50% is delayed by up to 0.99°CA, and the peak HRR decreases by up to 7.8% (13 J/°CA) (at SOI of -10, -15, and -15°CA ATDC, respectively) compared to non-EGR cases.

Notably, the changes in combustion speed as compared to no-EGR cases are insignificant for premixed combustion runs. The highest maximum pressure rise rate (MPRR) of 12 bar/°CA occurs at SOI of -35°CA regardless of EGR rate.

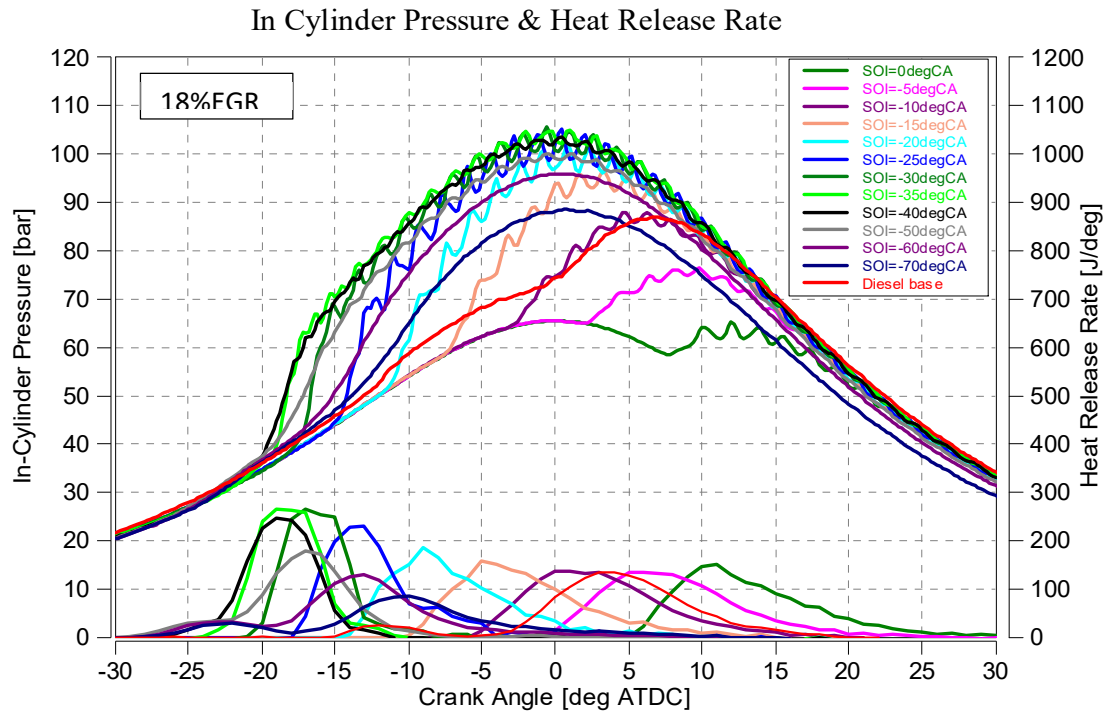


Figure 3.4: ICP and HRR histories according to °CA ATDC for various SOI timings in SMIS with 18% EGR.

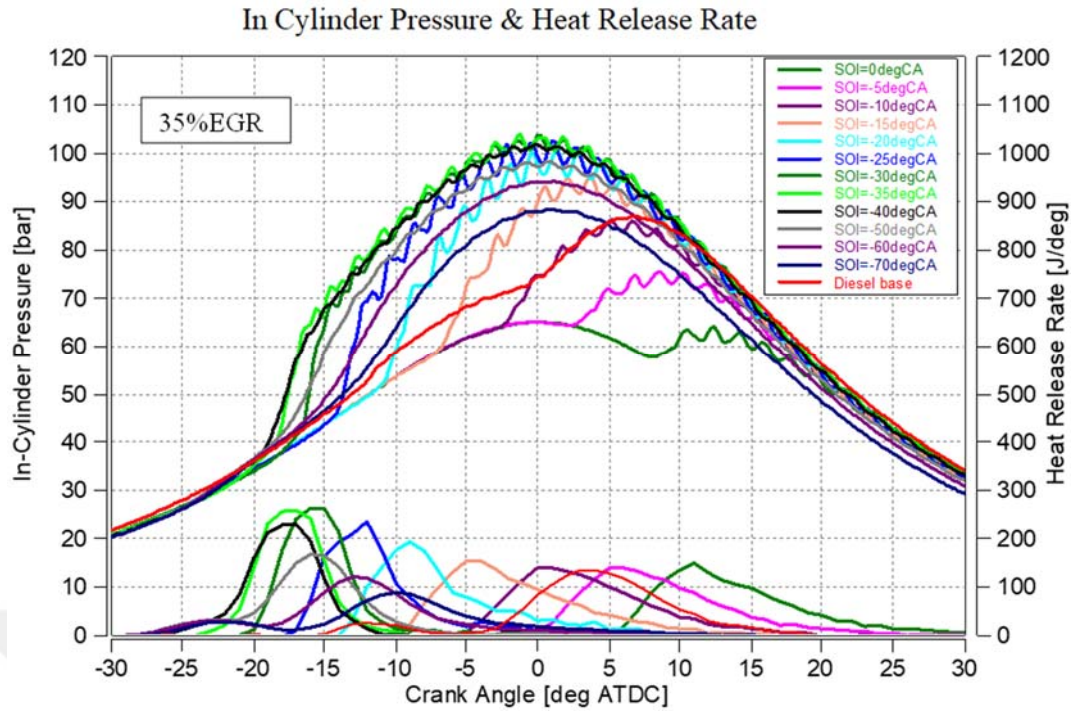


Figure 3.5: ICP and HRR histories according to °CA ATDC for various SOI timings in SMIS with 35% EGR.

The effect of SOI on NO_x emissions in SMIS at various EGR rates is shown in **Figure 3.6**. In diffusion-controlled combustion, NO_x emissions have a notable rise as the SOI is advanced from TDC to 30° before top dead center (BTDC).

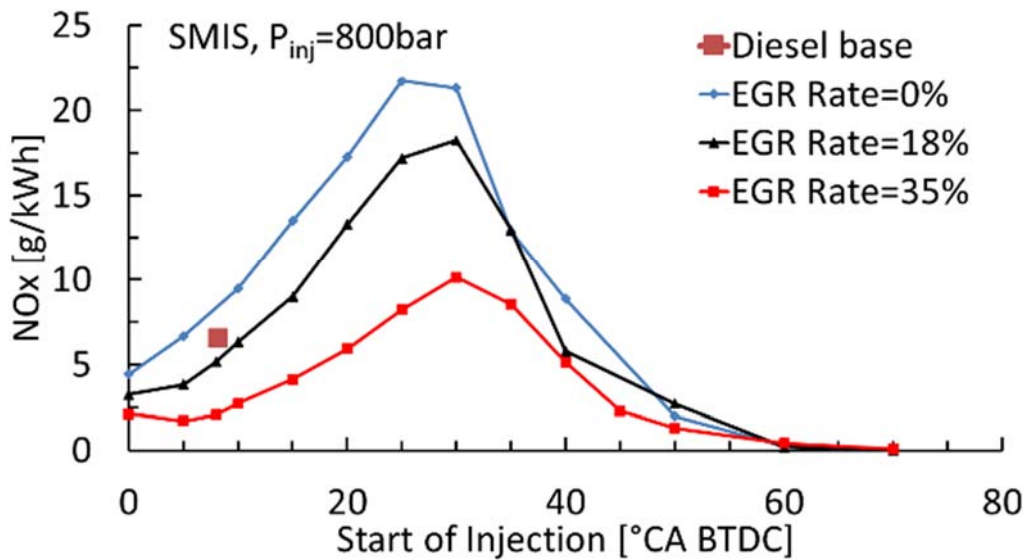


Figure 3.6: Engine-out NO_x emissions according to SOI for various EGR rates in SMIS.

As SOI is advanced, the emissions of NO_x decrease. NO_x emissions reach very low levels in the region of highly premixed combustion, where the SOI ranges between 45° and 70°CA BTDC . When the SOI is between 60° and 70°CA BTDC , the NO_x emissions are almost zero because of incomplete combustion caused by wall wetting. In the case of diffusion-controlled combustion, high EGR rates further reduce NO_x emissions. However, in highly premixed combustion cases, the NO_x emission levels are similar for the EGR rates of 0%, 18%, and 35% that were considered in this study.

Figure 3.7 shows the impact of SOI on both Indicated Specific Fuel Consumption (ISFC) and IMEP for different EGR rates in SMIS. The results demonstrate a significant increase in ISFC for advanced injections due to an earlier MFB50%. The optimal MFB50% for CDC is found to be between $2\text{--}4^\circ\text{CA ATDC}$, whereas for PCCI combustion, it is located between 10° to 20°CA BTDC . Notably, an SOI of -60°CA and -70°CA ATDC leads to a rapid increase in ISFC, coupled with a reduction in IMEP due to incomplete combustion caused by spray wall wetting. Furthermore, in cases where advanced injection is used without EGR, ISFC is reduced due to higher heat release rates compared to those with EGR.

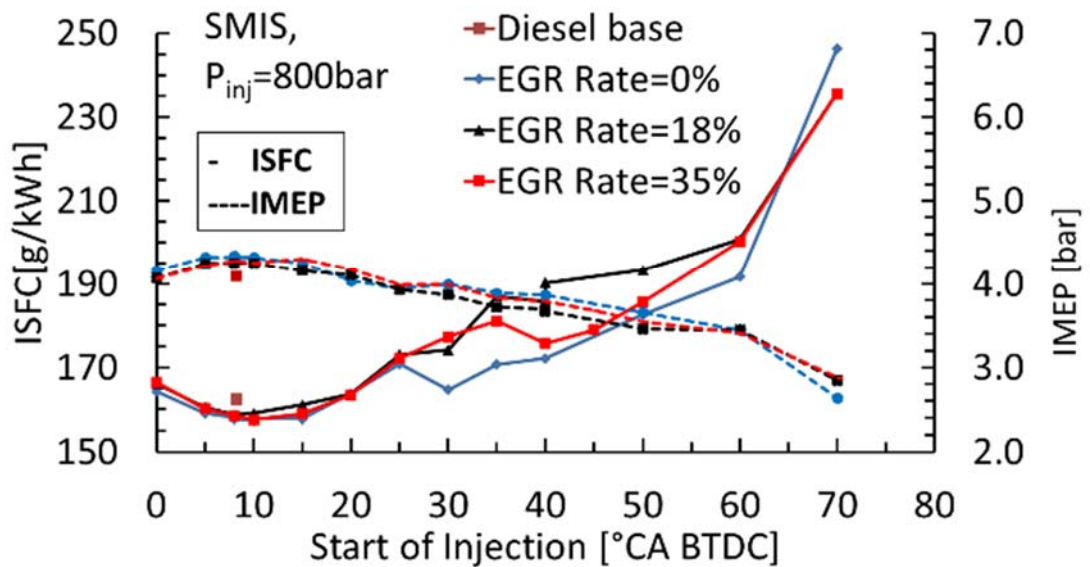


Figure 3.7: ISFC and IMEP according to SOI for various EGR rates in SMIS.

Effect of SOI on soot emissions for various EGR rates at 800 bar fuel injection system in single main injection strategy is plotted in **Figure 3.8**. Specifically, when the SOI was advanced to -60°CA and -70°CA ATDC in cases with advanced single injection,

soot emissions were higher compared to cases where the SOI was delayed. However, when 35% EGR was used, the soot emissions from highly premixed combustion of advanced single injection strategy were lower than those without EGR due to reduced spray penetration. Thus, higher EGR rates were found to be effective in reducing soot emissions by mitigating the problem of spray wall wetting in advanced single injection cases.

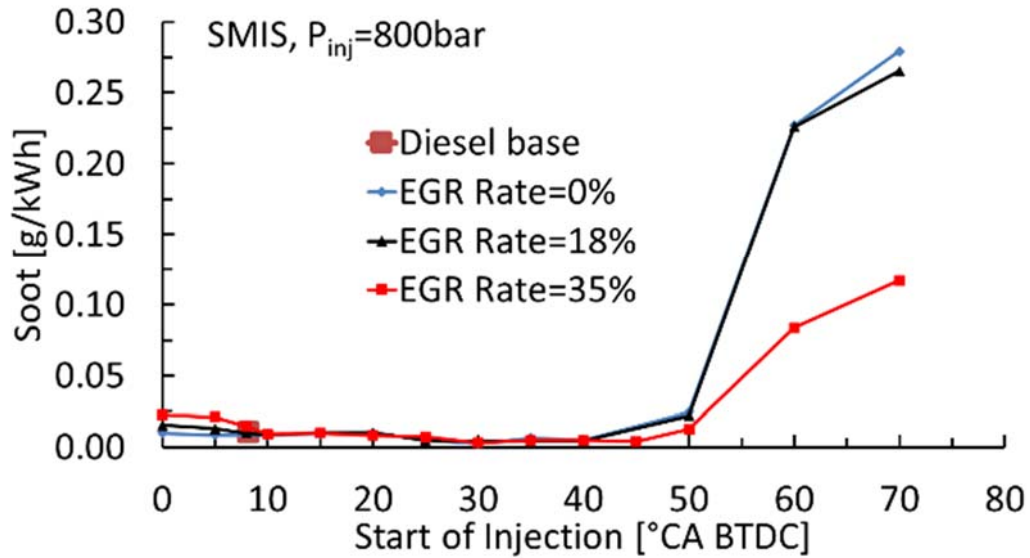


Figure 3.8: Engine-out soot emissions according to SOI for various EGR rates in SMIS.

The effect of SOI on UHC and CO emissions, at various EGR rates and 800 bar FRP in SMIS, is shown in **Figure 3.9** and **Figure 3.10**. UHC and CO emissions are higher in premixed low temperature combustion compared to diffusion-controlled combustion. This is because lower in-cylinder pressure and temperature during advanced injection resulting in decreased flame temperatures, leading to incomplete combustion. Additionally, UHC and CO emissions are increased due to spray cylinder wall impingement, which causes in-complete combustion of fuel in the liner zone and crevice volume. While EGR rate effects the spray penetration and soot emissions, CO and UHC emissions are not significantly influenced by EGR.

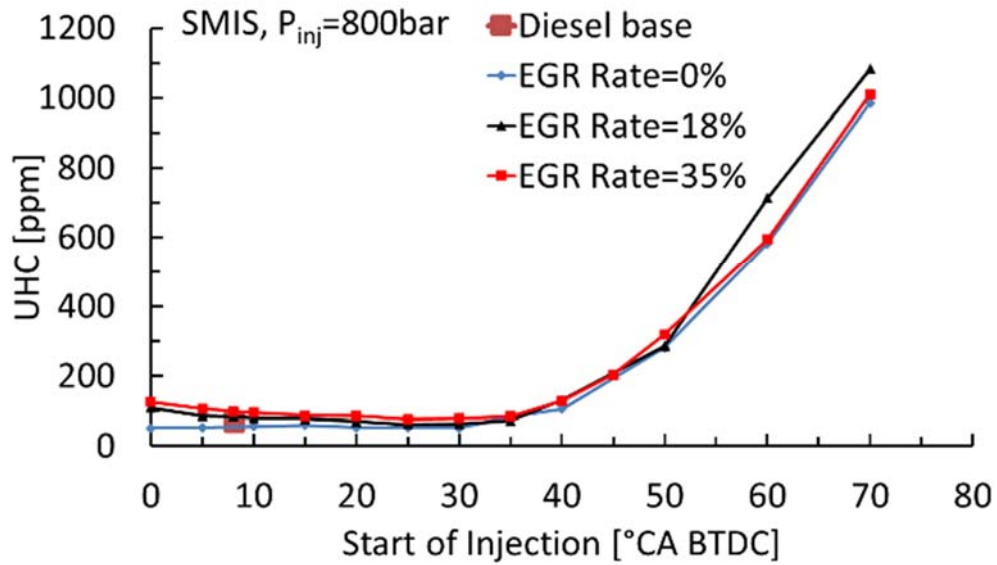


Figure 3.9: Engine-out UHC emissions according to SOI for various EGR rates in SMIS.

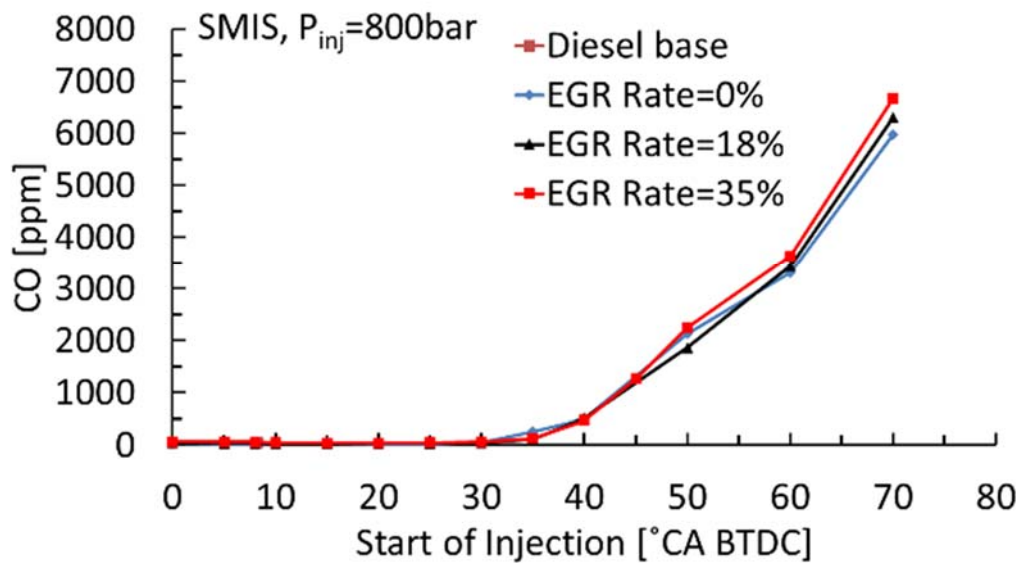


Figure 3.10: Engine-out CO emissions according to SOI for various EGR rates in SMIS.

Figure 3.11 shows the variation of ignition delay and MFB50% at different EGR rates at 800 bar fuel rail pressure according to SOI in single main injection strategy. Ignition delay remains relatively consistent, ranging slightly between 7.5°CA and 8°CA when SOI is advanced from 0°CA to -20°CA ATDC, that, MFB50% advances from 12°CA to -9°CA ATDC, resulting in stable combustion duration for conventional diesel

combustion with premixed and diffusion phases. As SOI is advanced further, ignition delay gradually increases due to the reduction of gas temperature and pressure, reaching 47.5°CA at SOI of -70°CA ATDC. Meanwhile, MFB50% advances until it reaches its minimum value of -18°CA ATDC at an SOI of -40°CA ATDC, then gradually retards to -11°CA ATDC at an SOI of -70°CA ATDC, as combustion delay increases significantly due to lower burn rates. For advanced SOI timings of 50 – 70°CA BTDC, fully low temperature combustion occurs, where ignition delay ranges between 25°CA and 47.5°CA and MFB50% approaches TDC (changing between -17°CA and -10°CA ATDC). Overall, EGR rate has a minor effect on ignition delay and MFB50%.

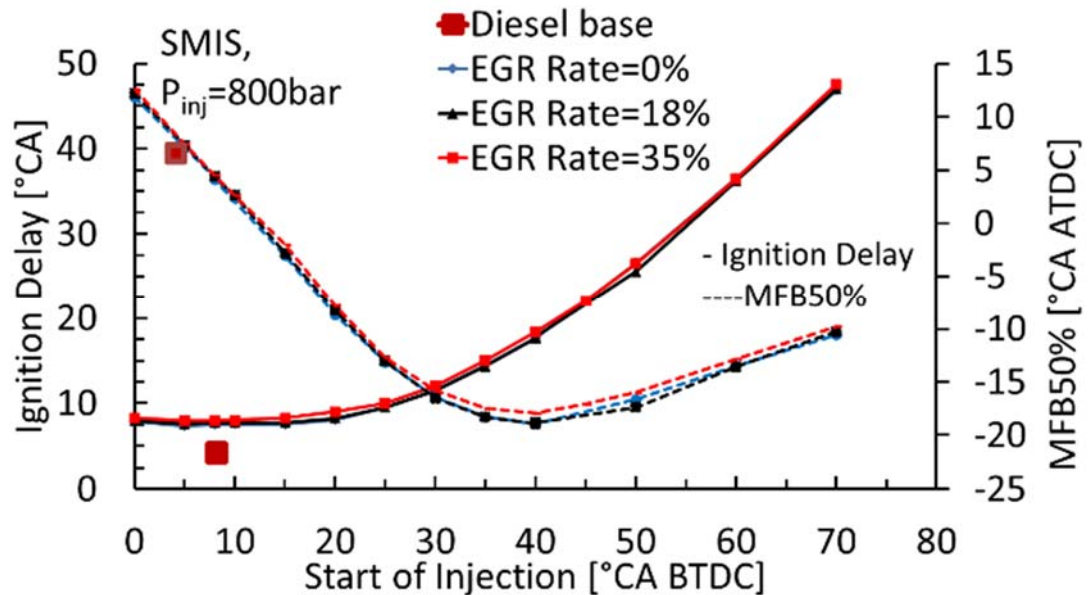


Figure 3.11: Ignition delay and MFB50% according to SOI for various EGR rates in SMIS.

3.4.3. Multiple Injection Strategy

In this section, the use of multiple injection strategies is explored as a means of avoiding incomplete combustion and reducing emissions of spray wall wetting. The study compares engine performance and emissions in different SMIS and DIS configurations, as well as TIS (Triple Injection Strategy) with sequential injection timings. Splitting the fuel into two or three injections can improve fuel-air mixing quality and reduce elevated emissions caused by longer spray penetration and wall wetting.

The findings suggest that split injection strategies can be an effective means of reducing emissions and improving engine performance in PCCI combustion [83], [108].

In this section, engine performance and emissions in SMIS with SOI of 60°CA, 50°CA and 40°CA BTDC, DIS with early SPI-SMI pair of 60°CA and 50°CA BTDC, as well as 60°CA and 40°CA BTDC, both respectively, and TIS with sequential early SOI timings (SPI, SMI and SPOI) of 60°CA, 50°CA and 40°CA BTDC are compared for various EGR rates. In DIS, one third and two thirds of the fuel mass is directly delivered into the cylinder during pilot and main injection, respectively. In TIS, one third of the fuel mass is directly supplied in each of the pilot, main and post injections.

Figure 3.12 shows the NO_x emissions for SMIS, DIS, and TIS with varying EGR rates up to 45%. It is observed that SMIS with SOI of 40°CA BTDC produces the highest NO_x emissions for any EGR rate. However, DIS and TIS can achieve NO_x emissions below 2 g/kWh for EGR rates above 40%. Notably, DIS with SPI-SMI pair of 60°CA and 40°CA BTDC exhibits the most significant reduction in NO_x emissions with increasing EGR rate.

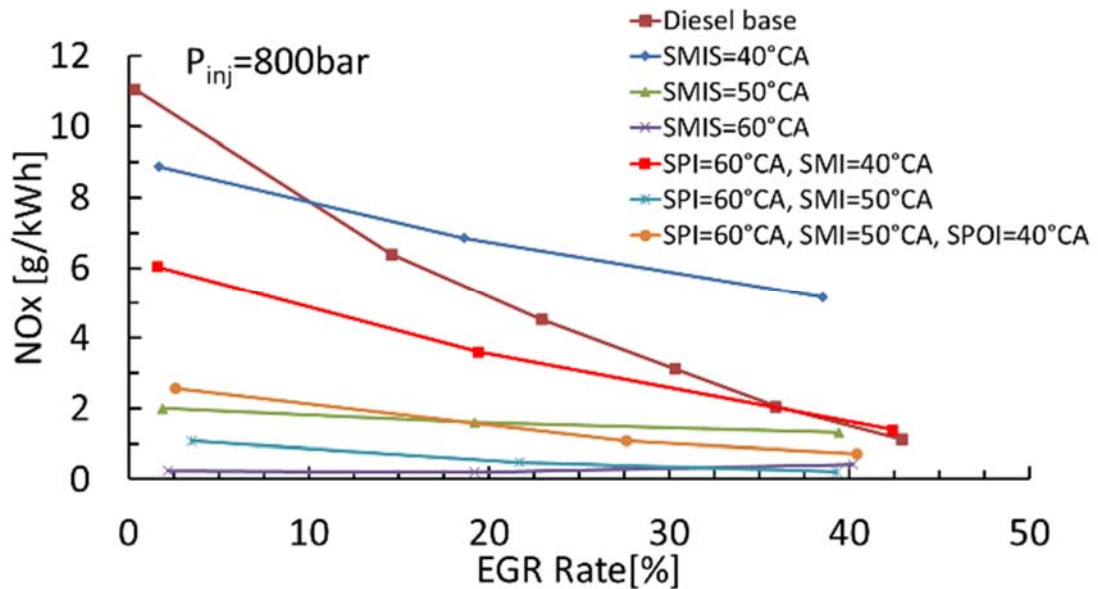


Figure 3.12: NO_x emissions of injection strategies with various early injection timings according to EGR rate.

Figure 3.13 indicates that soot emissions are less than 0.05 g/kWh in all cases except for SMIS with SOI of 60°CA BTDC. However, the risk of spray wall wetting can be eliminated by implementing split injection cases with SPI of 60°CA BTDC and for SMIS cases with SOI later than 50°CA BTDC. Interestingly, heavy EGR can reduce/eliminate the risk of wall wetting for advanced injection strategies.

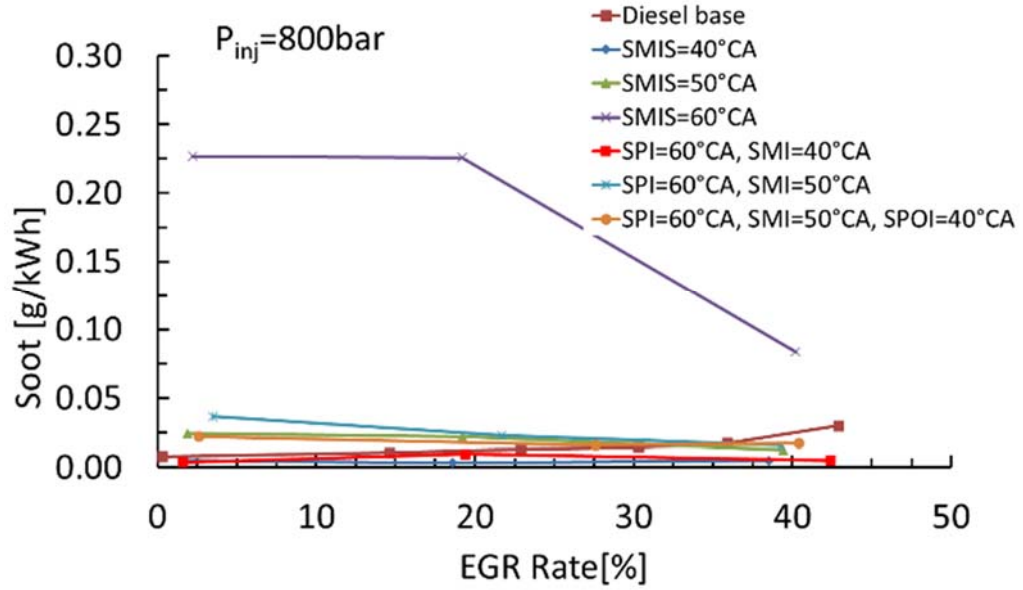


Figure 3.13: Soot emissions of injection strategies with various early injection timings accordingly to EGR rate.

Lowest ISFC is obtained by DIS with SPI-SMI pair of 60°CA and 40°CA BTDC for a 42.3% EGR rate is shown in **Figure 3.14**.

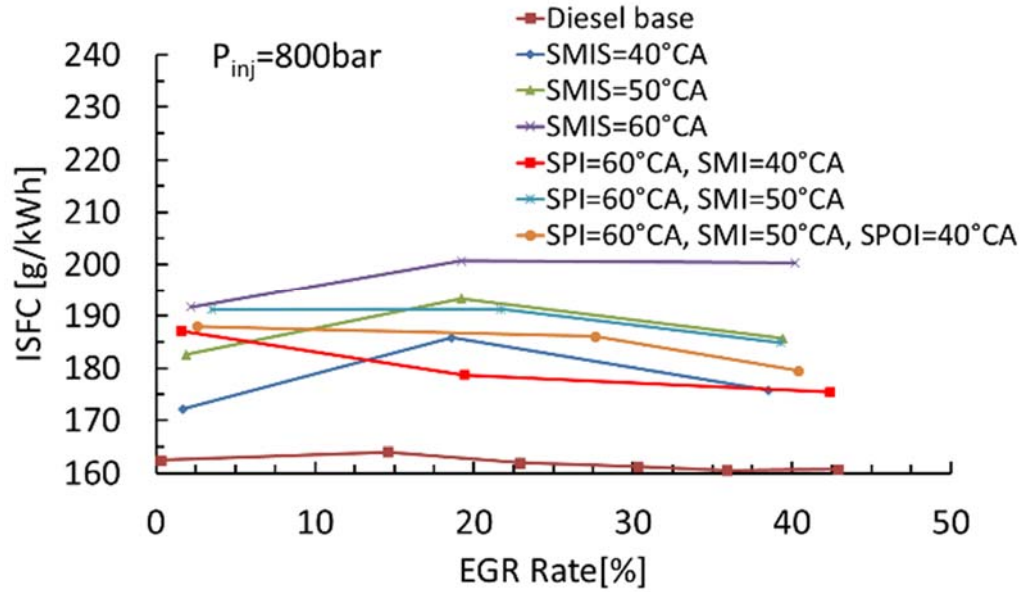


Figure 3.14: ISFC of injection strategies with various early injection timings according to EGR rate.

The effects of injection strategies and timings on UHC and CO emissions in base Diesel and PCCI cases under various EGR rates at 800 bar FRP are investigated. The results, as shown in **Figure 3.15** and **Figure 3.16**, indicates that the highest UHC and CO emissions were observed in early SMIS when the SOI was set at 60°CA BTDC due to incomplete combustion caused by wall wetting. On the other hand, the lowest UHC and CO emissions in early SMIS were achieved when the SOI was set at 40°CA BTDC, which prevented spray wall wetting and resulted in more uniform fuel air mixture formation. Furthermore, this approach enabled the gas pressure and temperature to reach higher levels at the SOI compared to more advanced injection cases.

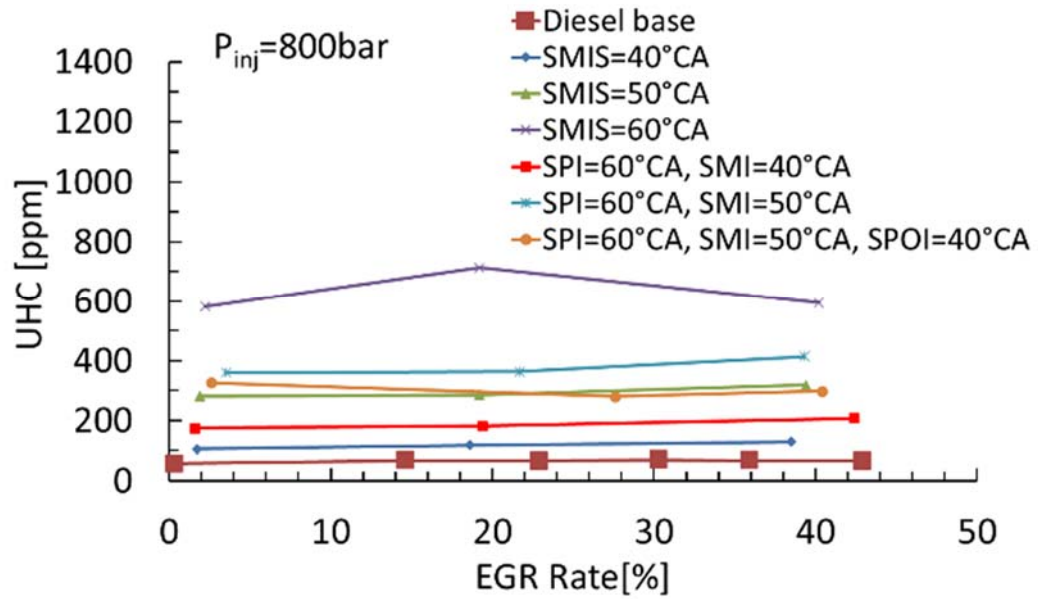


Figure 3.15: UHC emissions of injection strategies with various early injection timings according to EGR rate.

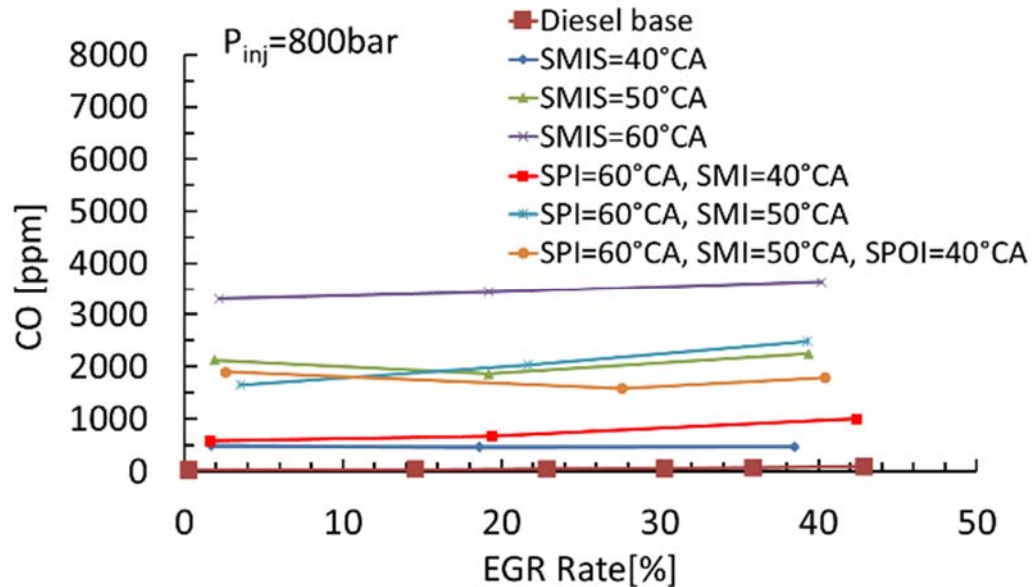


Figure 3.16: CO emissions of injection strategies with various early injection timings according to EGR rate.

The combustion and heat transfer efficiencies of Diesel engines are measured using different processes, and research by Stanton (2013) and Heywood (2018) has defined these processes [23], [109]. **Figure 3.17** shows the combustion efficiency of conventional diesel and PCCI combustion with different injection methods and

timings, based on the rate of EGR used. The highest efficiencies, ranging from 99.4% to 99.57%, were achieved in Diesel base cases. When using SMIS with an SOI of 60°CA BTDC and a 40% EGR rate, the efficiency improved from 84.2% to 89.8% due to reduced spray wall wetting and improved fuel air vapor mixture uniformity. The highest efficiencies, ranging from 96.8% to 97.1%, were obtained in DIS with an SPI-SMI pair of 60°CA and 40°CA BTDC in EGR rate sweeps of PCCI cases.

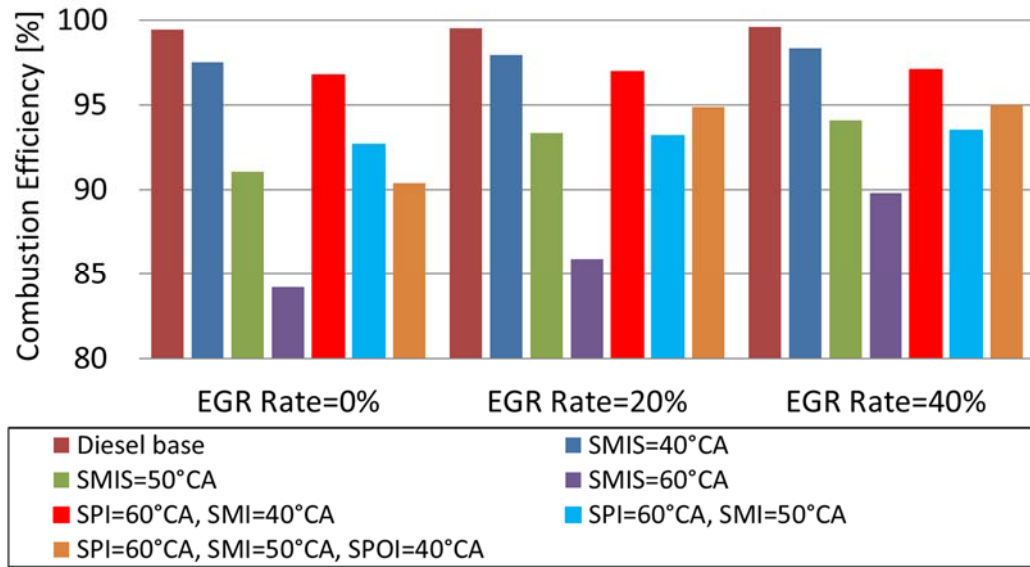


Figure 3.17: CE of various injection strategies and timings according to EGR rate.

The efficiency of heat transfer for Diesel and PCCI cases with various injection strategies and timings, on various EGR rates, are shown in **Figure 3.18**. The lowest heat transfer efficiencies occur at 20% EGR rate for advanced injection timings of SMIS with SOI of 60°CA, 50°CA, 40°CA BTDC, and early TIS. However, in DIS with SPI-SMI pair of 60°CA and 40°CA BTDC, heat transfer rate increases significantly with an increase in EGR rate. This is due to a decrease in HRR, combustion temperature, and therefore heat transfer rate to the cylinder wall, as EGR rate is increased.

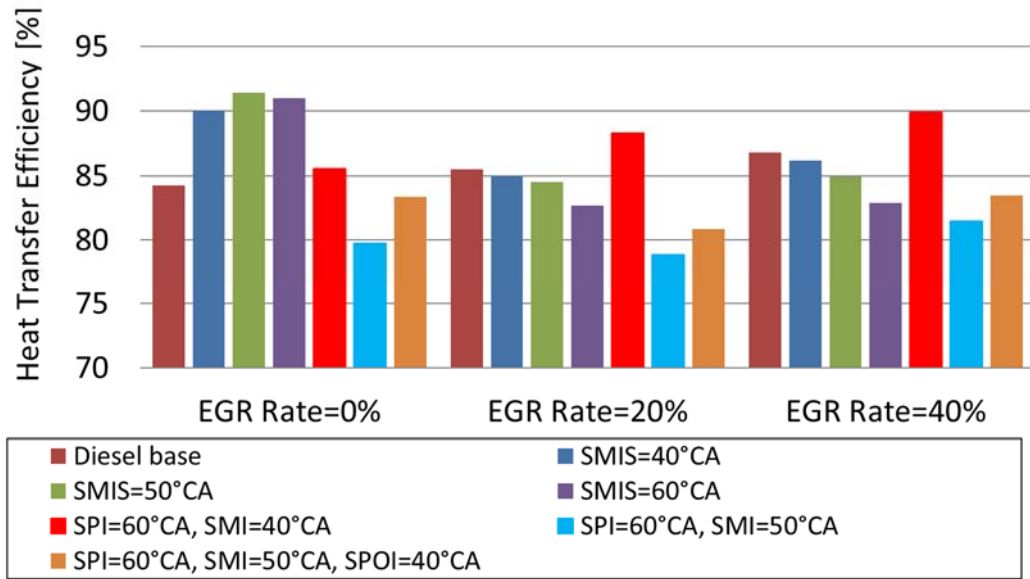


Figure 3.18: Heat transfer efficiency of various injection strategies and timings according to EGR rate.

Figure 3.19 presents a variety of injection strategies and timings for MFB50% of base Diesel and PCCI cases, with consideration to EGR rate at 800 bar FRP. The CDC performs the highest IMEP when MFB50% is around 4°C ATDC. Conversely, PCCI cases results MFB50% before TDC, as combustion occurs during the compression stroke at advanced injection timings, resulting in significant IMEP losses. Application of EGR results in a longer ID and reduced HRR. Based on the experimental findings, MFB50% can be delayed by a maximum of 2.6°C for a 40% EGR rate in PCCI combustion.

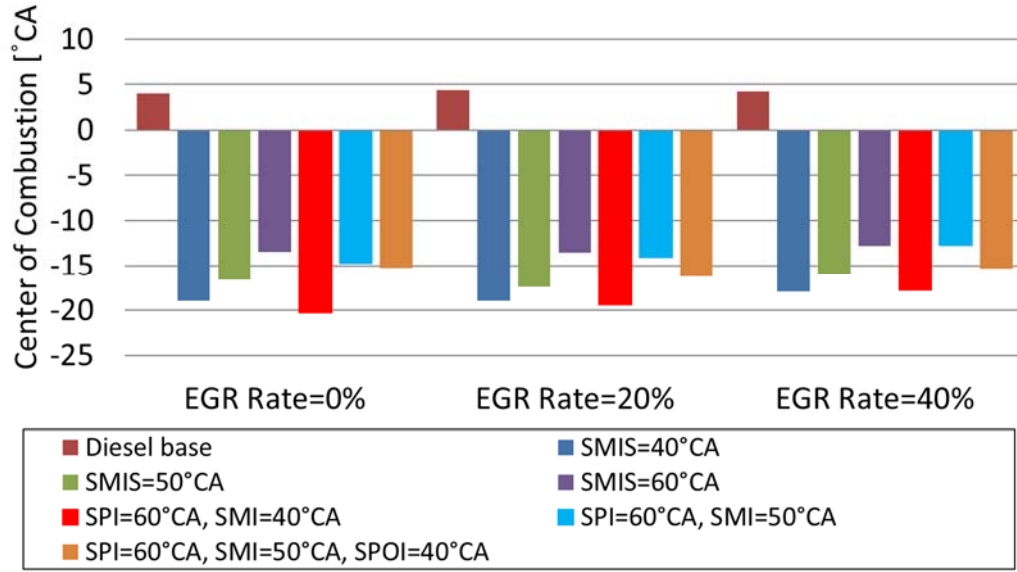


Figure 3.19: MFB50% of various injection strategies and timings according to EGR rate.

Moreover, when injection timings are advanced, an increase in EGR rate leads to a longer ignition delay, combustion starts in elevated in pressure and temperature, resulting in a significant increase in combustion efficiency. This phenomenon is particularly noticeable in SMIS cases with a start of injection of 50°CA or 60°CA BTDC, as well as early TIS. On the hand, in case of SMIS with a start of injection of 40°CA before top dead center and DIS with an SPI-SMI combination of 60°CA and 40°CA before top dead center, the impact of EGR rate on combustion efficiency is relatively minor. **Figure 3.20** shows the comparative CCE of different injection strategies and timings for both base Diesel and PCCI cases at 800 bar FRP, with DIS and an SPI-SMI combination of 60°CA and 40°CA before top dead center for a 40% EGR rate demonstrating the highest CCE of 47.52% among the considered injection strategies. This case also boasts a heat transfer efficiency of 97.1%, exceeding that of CDC at 89.9%, and an MFB50% of -17.8 °CA ATDC, resulting in the lowest ISFC of all the considered injection strategies.

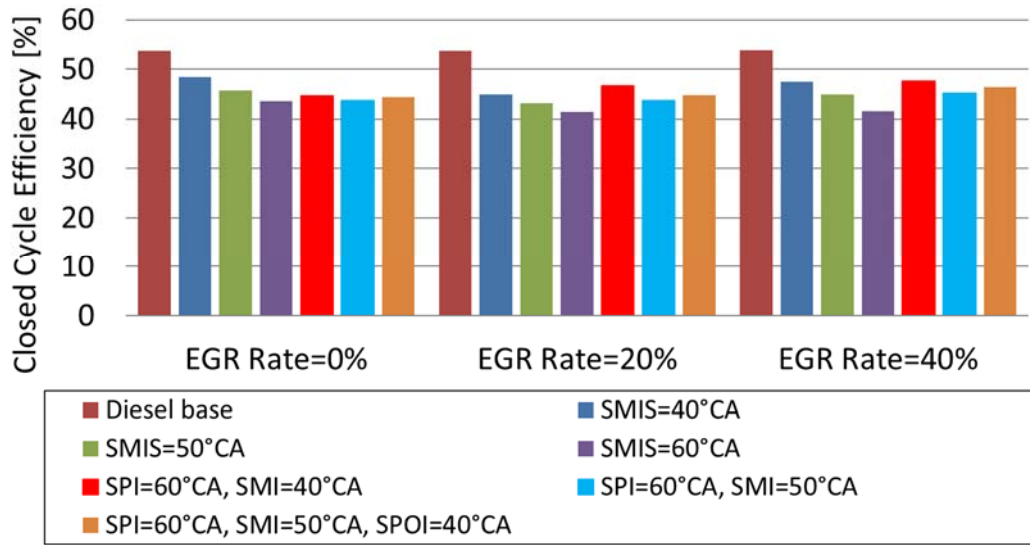


Figure 3.20: CCE of various injection strategies and timings according to EGR rate.

The results indicate that a DIS with a SPI-SMI pair of 60°CA and 40°CA BTDC, combined with an EGR rate of 42.3%, led to similar NO_x emissions without spray wall impingement, improved ISFC, and the lowest UHC and CO emissions compared to early SMIS, DIS, and TIS operations. Hence, the experimental investigation in the subsequent sections examines the effects of SPI-SMI pair of DIS and EGR rate in a wide range on the test engine.

3.4.4. Double Injection Strategy (DIS) with no-EGR

In the experiments, one third and two thirds of the fuel mass is delivered into the cylinder during the pilot and main injection, respectively. To prevent the subsequent injection events from interacting with each other, it is necessary to have a sufficient time lag between the injector closing and opening at the end and beginning of the pilot and main injections, respectively. Therefore, a minimum lag of 5 degrees of CA is maintained between the sequential injection events in DIS. In the experiments, the start of the pilot injection SPI occurred between 60°CA and 20°CA BTDC, followed by a SMI sweep with intervals of 5°CA to 10°CA up to TDC.

ICP and HRR histories according to °CA ATDC for early DIS with SPI of 60° and SMI sweep of -50, -40, -30, -20, -15, -10, -5, and 0°CA ATDC are presented in **Figure 3.21**. If the time lag between two early injections is small (for instance, DIS with SPI-

SMI pair of 60°CA and 50°CA BTDC, respectively), ID with respect to SPI timing is 37°CA, SOIgn is 23°CA BTDC, MFB50% is 16.5°CA BTDC and combustion duration (CD) is 13°CA and incomplete low temperature combustion due to wall wetting of the main injection results in low NO_x emissions of 1 g/kWh. As the time lag of early DIS is increased, (for instance, DIS with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively), ID with respect to SPI timing is 35°CA, SOIgn is 25°CA BTDC, MFB50% is 21°CA BTDC and CD is 8°CA and NO_x emissions increase to 6 g/kWh due to improved higher temperature combustion with shorter CD in accordance with less wall wetting by the main injection. Within the moderate injection time lag region (for instance, DIS with SPI-SMI pair of 60°CA and 30°CA BTDC, respectively), wall wetting by the main injection is avoided, ID with respect to SPI timing is 40°CA, SOIgn is 20°CA BTDC, MFB50% is 17.5°CA BTDC and CD is 5°CA and NO_x emissions peak to 18 g/kWh due to shortest CD and highest peak HRR thereof combustion temperature as fuel vapor air mixture (FVAM) auto-ignition 11°CA after SMI combusts both injected fuels simultaneously. In late main injection (for instance, DIS with SPI-SMI pair of 60°CA and 10°CA BTDC, respectively), without wall wetting by the main injection, ID with respect to SPI timing is 46.5°CA, SOIgn is 13.5°CA BTDC, MFB50% is 1.5°CA ATDC and CD is 30°CA and NO_x emissions decrease to 8 ppm. MFB50% which is delayed after TDC increases as SMI approaches TDC so that NO_x emissions further decrease to 4 g/kWh for SMI of 0°CA due to decreasing temperature of much longer combustion in expansion stroke with ID with respect to SPI timing of 47.5°CA, SOIgn of 12.5°CA BTDC, MFB50% of 11.5°CA ATDC and CD of 48°CA. Pilot injection with SPI of 60°CA BTDC auto-ignites before SMI if SMI is closer to TDC than 13°CA BTDC.

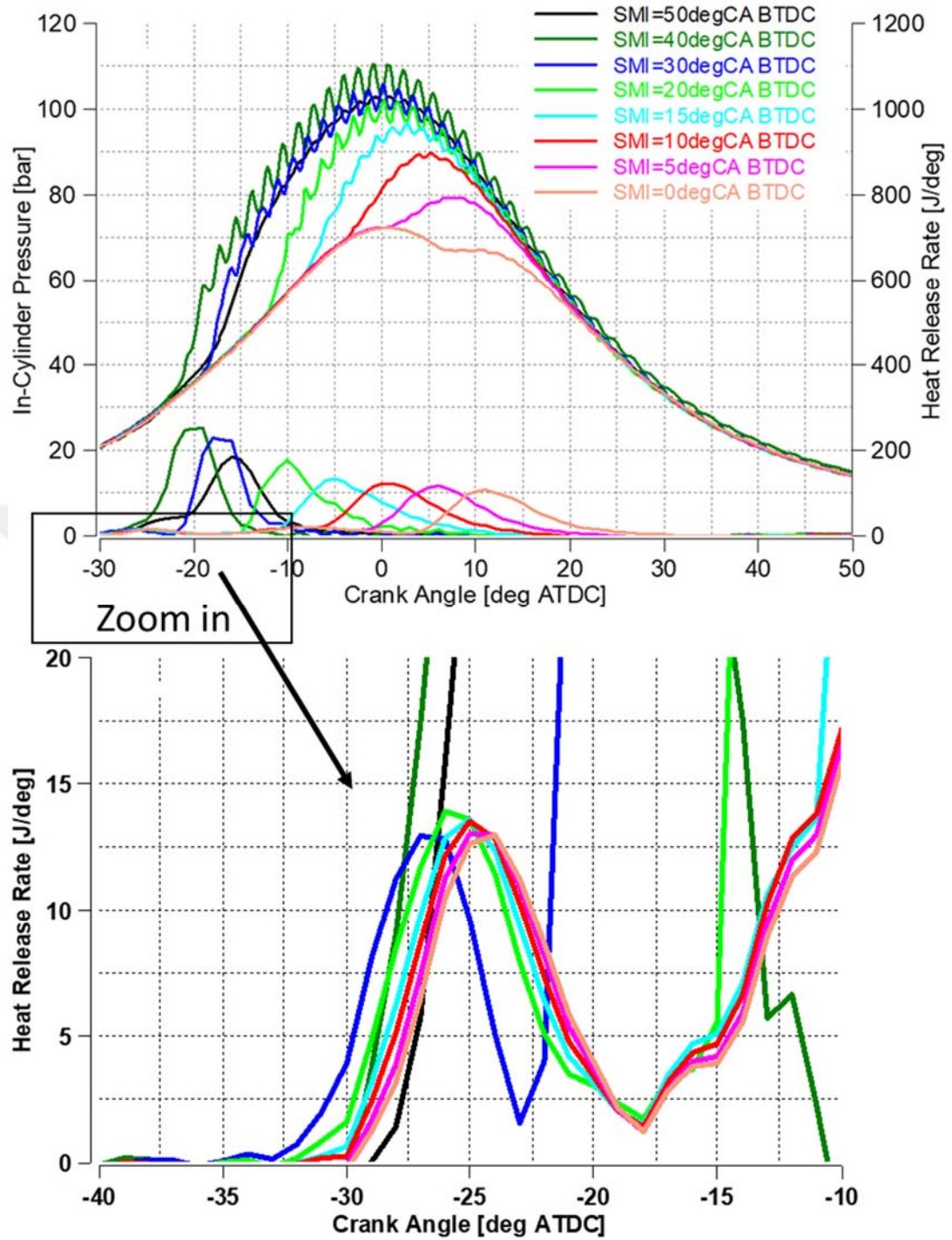


Figure 3.21: ICP and HRR histories according to °CA ATDC for early DIS with SPI of 60° and SMI sweep of -50, -40, -30, -20, -15, -10, -5, and 0°CA ATDC.

NO_x emissions according to SMI for various SPI timings are compared with those of base Diesel case and SMIS sweep, at 800 bar FRP with no-EGR in **Figure 3.22**. The results showed that DIS reduced NO_x emissions compared to SMIS for early injection

timings ranging between -60°CA and -40°CA ATDC and base diesel case. Increasing the time lag between pilot and main injection initially increased NO_x emissions, but eventually decreased after reaching a peak at around -30°CA ATDC for both DIS and SMIS strategies.

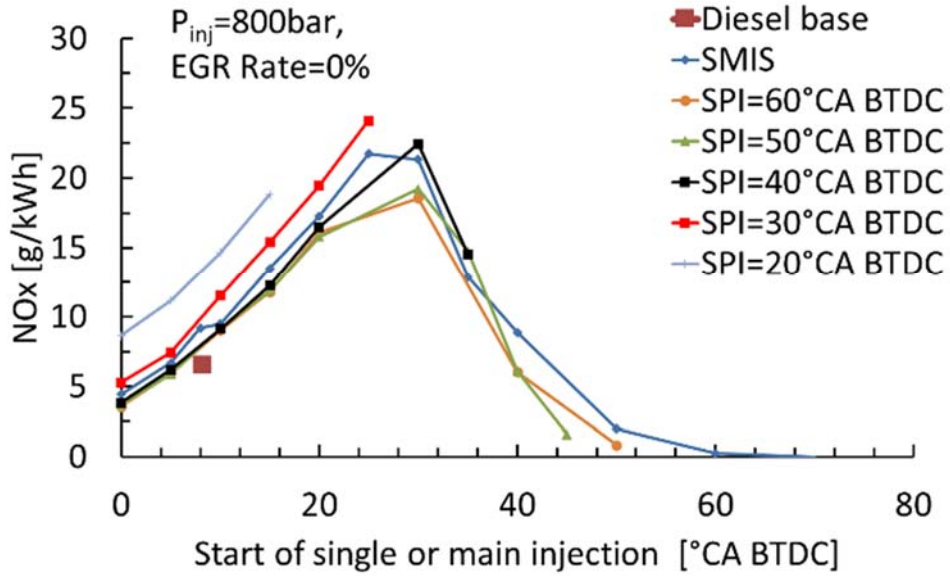


Figure 3.22: NO_x emissions of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

When using late DIS sweeps with spilt pilot injection of -30°CA and -20°CA ATDC, the timing of the first injection auto-igniting before the SMI depends on the proximity of the SMI to TDC. If the SMI is closer to TDC than 17.2°CA BTDC and 11.5°CA BTDC, respectively, main combustion occurs at higher temperatures with higher HRR compared to late SMIS with the same SOI as SMI. However, MFB50% is delayed as SMI approaches TDC, occurring after TDC if SMI is after 8°CA BTDC and 10°CA BTDC, respectively. NO_x emissions decrease as SMI is delayed due to decreasing temperature in the expansion stroke but are still higher than those of SMIS with the same SOI as SMI due to higher diffusion combustion temperatures. In late DIS cases, soot, UHC, and CO emissions are like the base Diesel case due to diffusion combustion of the first and second injected fuels.

In summary, the use of DIS with SPI-SMI pairs of 60°CA and 50°CA BTDC, and 50°CA and 45°CA BTDC, respectively, results in a significant reduction of NO_x

emissions by 1 g/kWh and 2 g/kWh compared to base Diesel combustion and SMIS with SOI of 50°CA and 45°CA BTDC. The NO_x emissions for these latter cases were found to be 3.5 g/kWh, 2.5 g/kWh, and 6 g/kWh, respectively. These results suggest that the use of DIS with specific injection timings can effectively reduce NO_x emissions in diesel engines.

In **Figure 3.23**, ISFC values according to SMI for various SPI timings are compared to those of the base Diesel case and SMIS sweep, at 800 bar FRP with no-EGR. The results show that ISFC for DIS with early SPI timings of 60°CA, 50°CA, and 40°CA BTDC are generally higher than that of SMIS with the same SOI timing as SMI, and they display an oscillatory trend as the SMI timing is varied up to TDC. However, slightly lower ISFC values are obtained for the DIS cases with SPI-SMI pairs of 60°CA and 50°CA BTDC, and 50°CA and 45°CA BTDC, respectively.

However, ISFC for DIS with retarded SPI timings of 30°CA and 20°CA BTDC is always higher than that of SMIS with the same SOI timing as SMI, as the SMI timing is delayed up to TDC. The ISFC of DIS with SPI timing of 30°CA BTDC first decreases and then increases, while that with SPI timing of 20°CA BTDC increases, as SMI is delayed up to TDC.

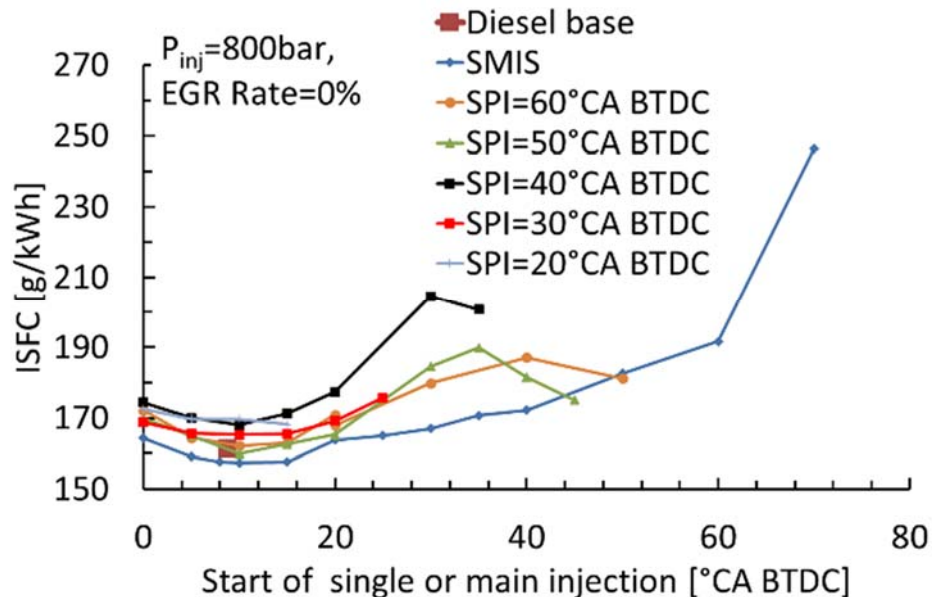


Figure 3.23: ISFC of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

Soot emissions of DIS with various SPI timings to that of the base Diesel case and SMIS sweep, at 800 bar FRP with no-EGR are compared in **Figure 3.24**. We observed that there were no significant soot emissions in any DIS, thanks to reduced wall wetting. In addition, the soot emissions in SPI-SMI pairs of 60°CA and 50°CA BTDC, and 50°CA and 45°CA BTDC cases were notably lower than those of the base Diesel and SMIS cases with the same SOI as SMI.

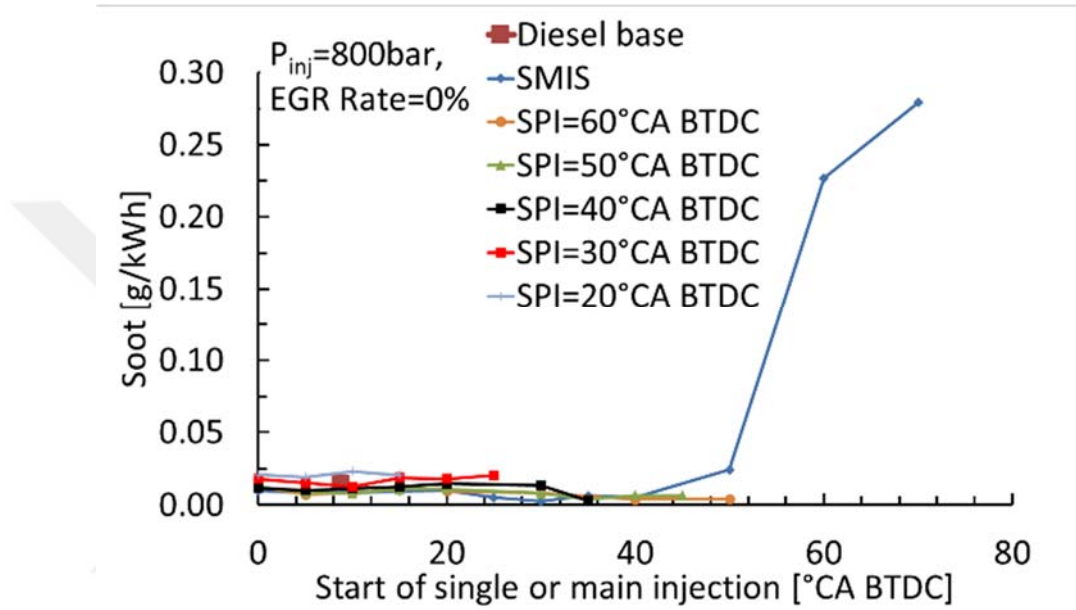


Figure 3.24: Soot emissions of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

UHC emissions of a DIS engine with SPI to a base diesel engine and a spark ignition with stratified charge (SMIS) engine at 800 bar fuel rail pressure without EGR are compared in **Figure 3.25**. The results showed that the UHC emissions of the DIS engine were higher than the base diesel engine and SMIS engine with the same SOI as SMI. As the SPI was advanced, the difference in UHC emissions between DIS and SMIS with the same SOI as SMI increased. However, there were minor differences in UHC emissions with DIS with SPI-SMI pairs of -60° and -50°CA ATDC, -50° and -45°CA ATDC, and -40° and -35°CA ATDC, as well as for any SPI of -20°CA ATDC case, and SMIS with the SOI as DIS.

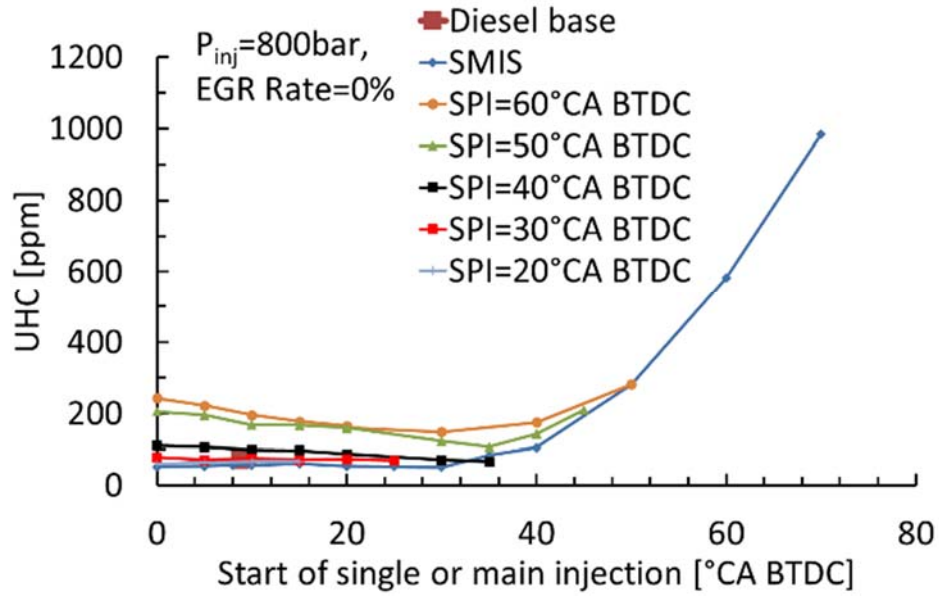


Figure 3.25: UHC emissions of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

In **Figure 3.26**, CO emissions of DIS with various SPI timings according to SMI for 800 bar FRP with no-EGR are compared to those of the base Diesel case and SMIS sweep. It was found that the CO emissions of DIS were slightly lower than those of SMIS with the same SOI as SMI for certain SPI-SMI pairs, including -60° and -50°CA ATDC, -50° and -45°CA ATDC, -50° and -40°CA ATDC, and -40° and -35°CA ATDC. However, for all SPI timings studied, CO emissions of DIS with SMI ranging from -30° to 0°CA ATDC were higher than those of SMIS with the same SOI as SMI. CO emissions of DIS were low and like those of SMIS with the same SOI as SMI for SPI timing of -20°CA. However, as SMI approached TDC, the CO emissions of DIS increased significantly for SPI timings between -60° and -30°CA ATDC due to incomplete combustion of the first injected fuel near the cylinder walls by the diffusion flame formed by the late main injection.

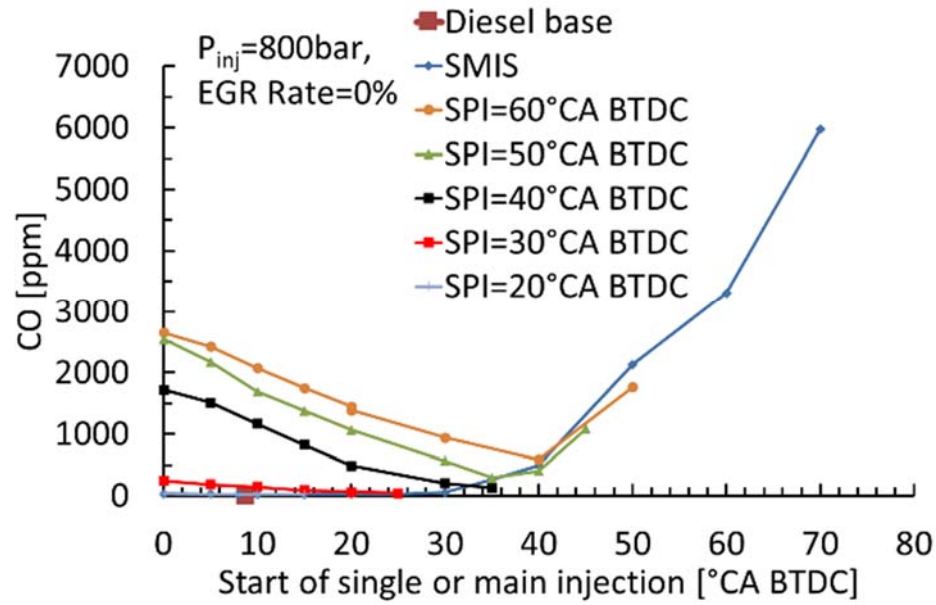


Figure 3.26: CO emissions of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

ID of SPI and MFB50% of DIS with respect to SMI for various SPI timings are shown in **Figure 3.27**. The results were compared with those of a base Diesel case and SMIS sweep at 800 bar FRP with no-EGR. ID of SMIS sweep with respect to Start of Injection (SOI) is plotted. It is found that if FVAM ignition occurs after SMI in DIS, the ID with respect to SMI is up to 7°CA shorter than that of SMIS with the same SOI as SMI. However, the differences between MFB50% of DIS and SMIS with the same SOI as SMI are minor in no-EGR operation.

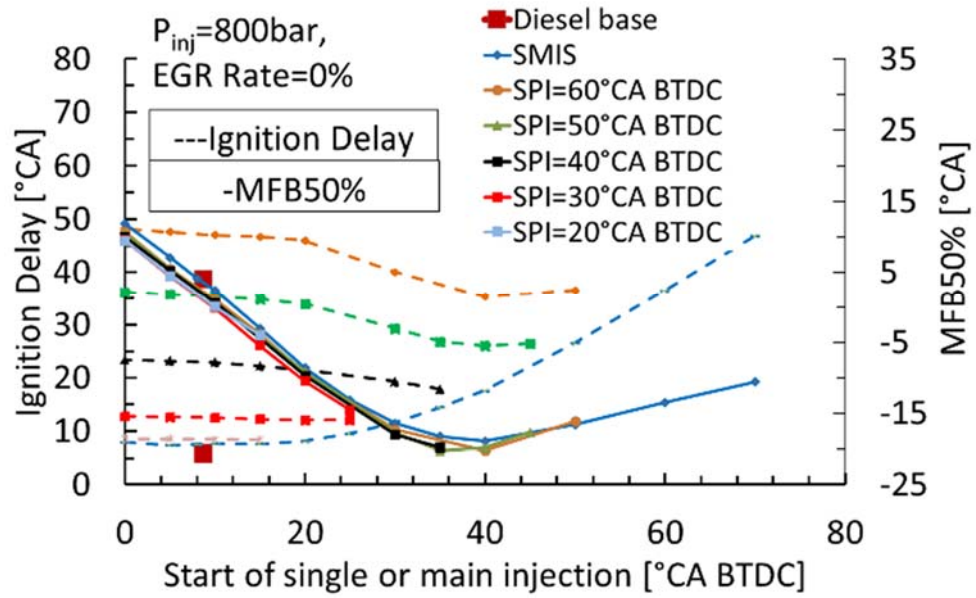


Figure 3.27: ID and MFB50% of DIS according to SMI for various SPI timings, base Diesel case and SMIS sweep with no-EGR.

The graphs in **Figure 3.28** are presenting ICP and HRR histories of SPI-SMI pairs with -60° and -50°CA ATDC and -50° and -40°CA ATDC at 800 bar FRP without EGR. When comparing early DIS and SMIS with the same SOI as SPI, it is evident that early DIS, both SOIgn and MFB50% advances, yields shorter CD and higher peak HRR and ICP due to improved FVAM uniformity.

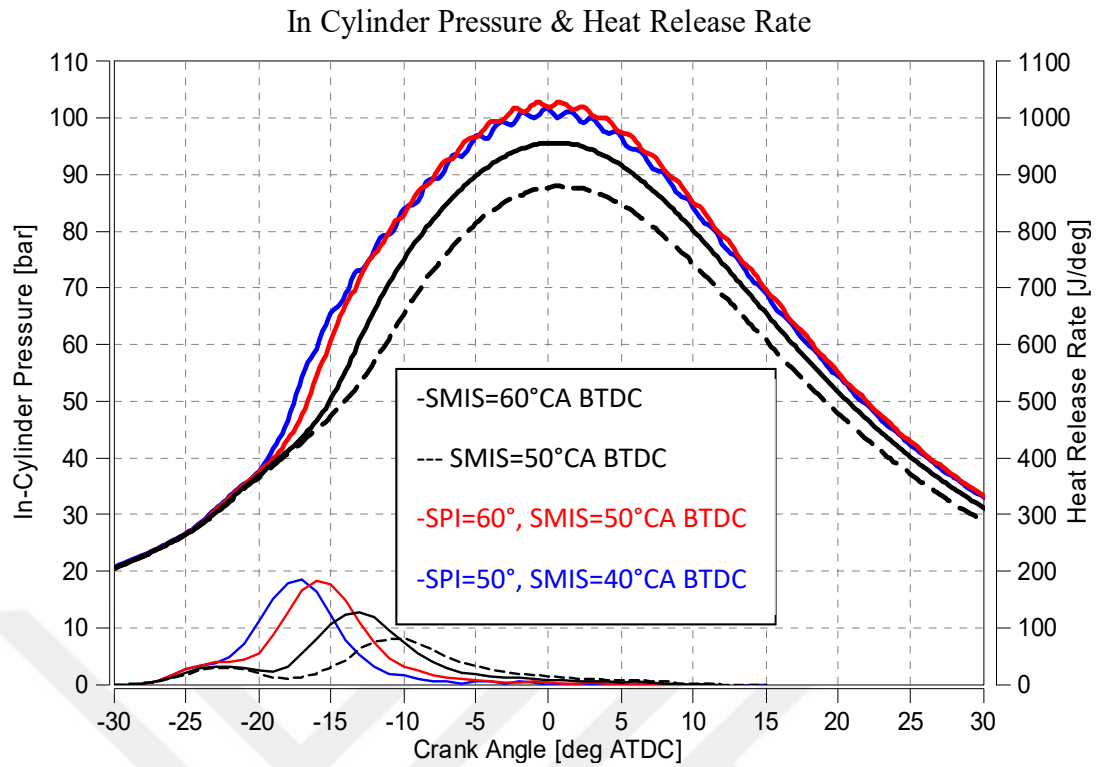


Figure 3.28: ICP and HRR histories according to °CA ATDC of early DIS and SMIS with the same SOI as SPI for SPI-SMI pairs of -60° and -50°CA ATDC, -50° and -40°CA ATDC without EGR.

3.4.5. Nitrous Double Injection Strategy (DIS) with Heavy EGR

Implementing early DIS in engines leads to improved uniformity of fuel vapor-air mixture and reduced wetting of cylinder walls by the spray. This is achieved by splitting the amount of injected fuel, which leads to shorter spray penetration lengths. Furthermore, low temperature combustion resulting from this approach significantly lowers NO_x emissions and reduces engine-out soot emissions below those achieved by base Diesel and SMIS, provided that the same SOI is used for SPI-SMI pairs of -60° & -50°CA ATDC and -50° & -40°CA ATDC, and the FRP is set at 800 bars without EGR.

However, in the case of the SPI-SMI pairs, (ISFC) is significantly higher than that of the base Diesel case, with a 12.3% increase for SPI and a 7.4% increase for SMI, as illustrated in **Figure 3.23**. This is because combustion occurs further away from top dead center (TDC), with a SOI_{Ign} of 23°CA and 24°CA before TDC, and a 50% mass fraction burn (MFB50%) of 16.5°CA and 18°CA before TDC, respectively. As a result, early direct injection without EGR is not suitable for low-load operation, as it

leads to excessive ISFC. An alternative approach to reducing NO_x emissions while maintaining acceptable soot emissions and without compromising ISFC is to delay SOIgn and MFB50% closer to TDC by implementing sufficient EGR rates.

In **Figure 3.29**, ICP and HRR histories according to °CA in early DIS with SPI of 60° and SMI of 40° BTDC are shown for different EGR rates of 0 to 14.1, 28.9, 48.4, 63.7, 70.0 and 75.1% respectively. The results indicate that EGR has a significant impact on ID, MFB50%, peak ICP, and peak HRR. Specifically, increasing the EGR rate from 0 to 75.1% results in a 16% (17.7 bar) decrease in peak ICP and a 47.2% (118.3J/°CA) decrease in peak HRR, accompanied by a delay of 7 °CA and 13.6°CA in SOIgn and MFB50%, respectively. **Table 3.5** summarizes the peak ICP, peak HRR, SOIgn, and MFB50% for different EGR rates.

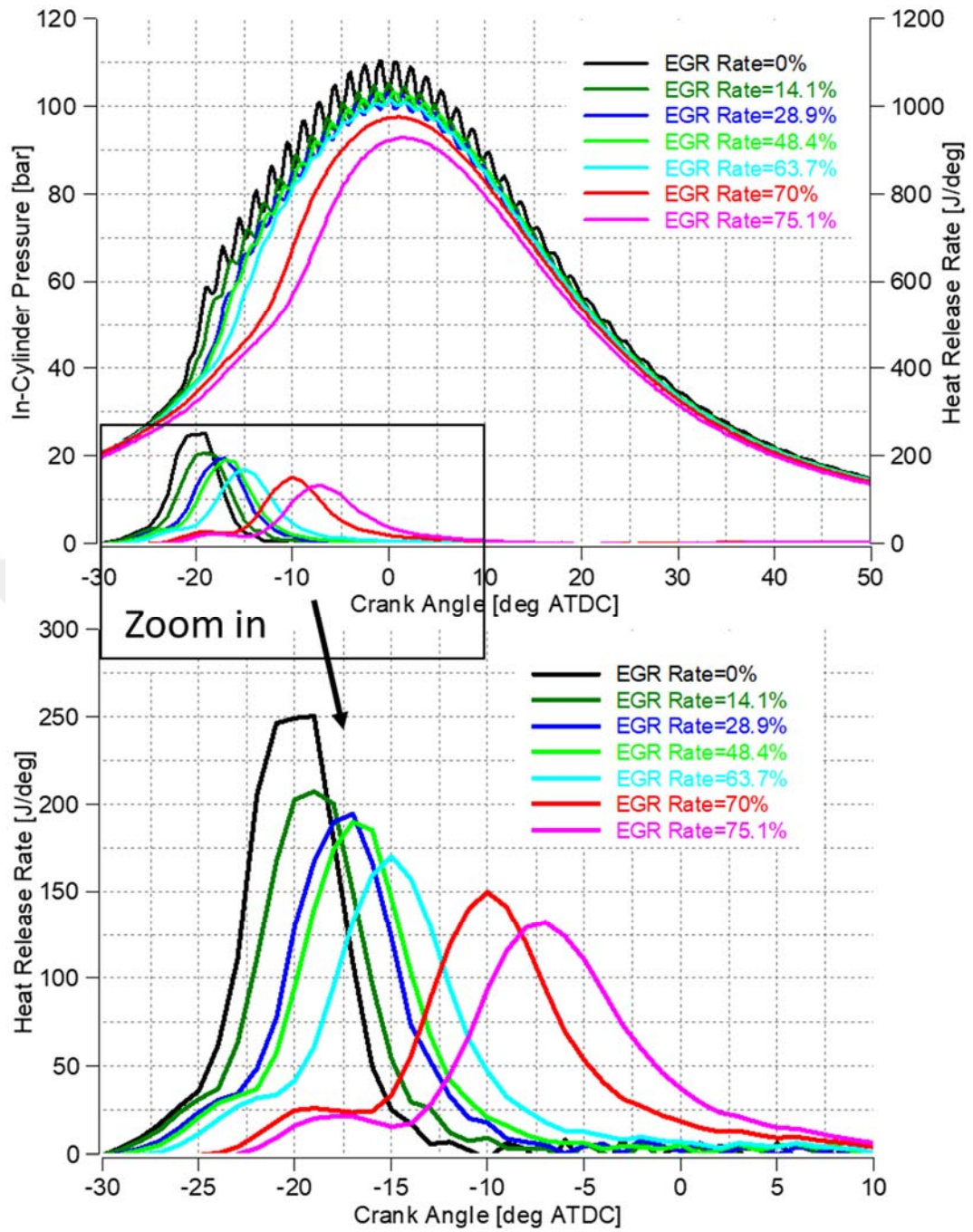


Figure 3.29: ICP and HRR histories according to °CA ATDC for various EGR Rates for CDC and DIS-PCCI operation with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively.

Table 3.5: Peak ICP, peak HRR, SOIgn and MFB50% for various EGR rates in early DIS with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively.

EGR rate	Peak ICP	Peak HRR	SOIgn	MFB50%
%	[bar]	[J/ °CA]	[°CA BTDC]	[°CA BTDC]
0	110.6	250.5	29.8	20.3
14.1	105.3	207.6	29.6	19.4
28.9	103.4	194.7	29.0	17.8
48.4	102.9	189.8	28.8	17.0
63.7	101.5	170.1	28.2	15.1
70.0	97.6	149.8	24.2	9.7
75.1	92.9	132.2	22.8	6.7

Up to 63.7% EGR rate, combustion of pilot injection starts between 29.8 and 28.2 °CA BTDC. Then, 5-7°CA after SOIgn, combustion of the main injection accelerates HRR. Combination of pilot and main combustion events results in peak HRR of 250.5 J/°CA in no-EGR case. However, for EGR rates of 70%, and 75.1%, IDs of the main injection are considerably higher than those of the lower EGR rate cases which cause a decreasing trend in HRR of the pilot injection after reaching a peak and then HRR increases rapidly as the main injection auto ignites.

Figure 3.30 displays the NO_x emissions for both CDC and PCCI operations with SPI-SMI pair of 60° and 40°CA BTDC, respectively, at 800 bar FRP. The results indicate that DIS-PCCI operation leads to a significant 45% reduction in NO_x emissions compared to CDC under no-EGR condition. With an increase in EGR rate, the engine-out NO_x emissions for both CDC and PCCI operation with DIS decrease rapidly. While NO_x emissions for DIS-PCCI combustion are lower than those of CDC for EGR rates up to 50%, the difference between them diminishes beyond this point. In contrast, the engine-out soot emissions for DIS-PCCI operation with 50% EGR rate (0.006 g/kWh) are only one-fifth of the CDC with the same EGR rate and approximately one-third of the base Diesel operation with 32% EGR rate (0.014 g/kWh). **Figure 3.31** displays the engine-out soot emissions for CDC and DIS-PCCI operation with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively, according to EGR rate. The results indicate that while soot emissions increase with EGR rate for CDC, they remain stable at a lower level for early DIS-PCCI operation with SPI-SMI pair of 60°CA and 40°CA BTDC. For EGR rates above 70%, both NO_x and soot emissions are negligible due to low temperature incomplete combustion.

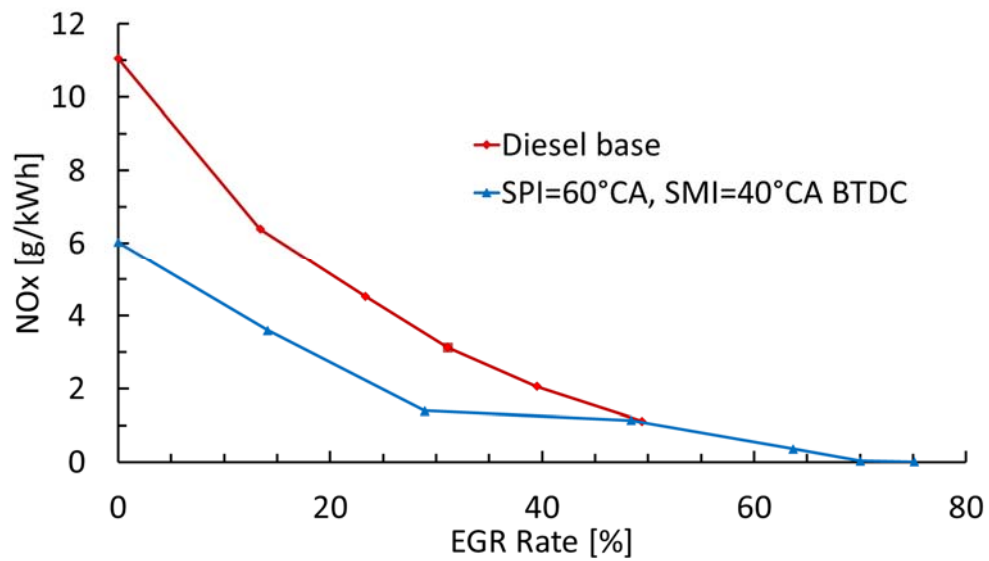


Figure 3.30: Comparison of engine-out NO_x emissions according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively.

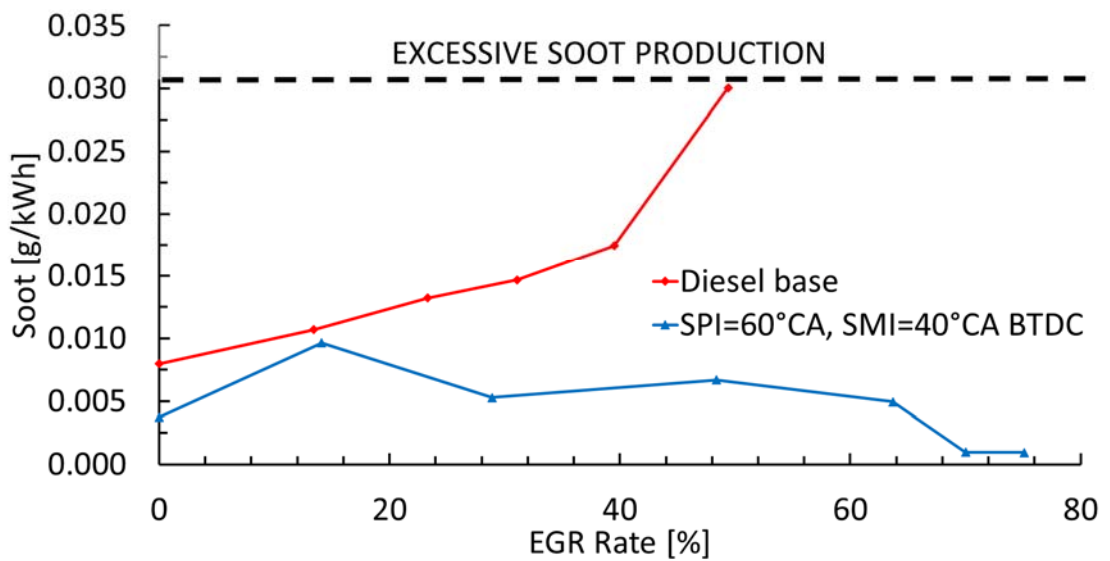


Figure 3.31 Comparison of engine-out soot emissions according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°CA and 40°CA BTDC, respectively.

Significant increase in UHC emissions in DIS-PCCI cases compared to CDC, with a ratio of three to four times higher for any EGR rate, as shown in **Figure 3.32**. Additionally, the research showed that UHC emissions increase considerably in DIS-

PCCI operation when the EGR rate exceeded 60%, which was due to incomplete combustion.

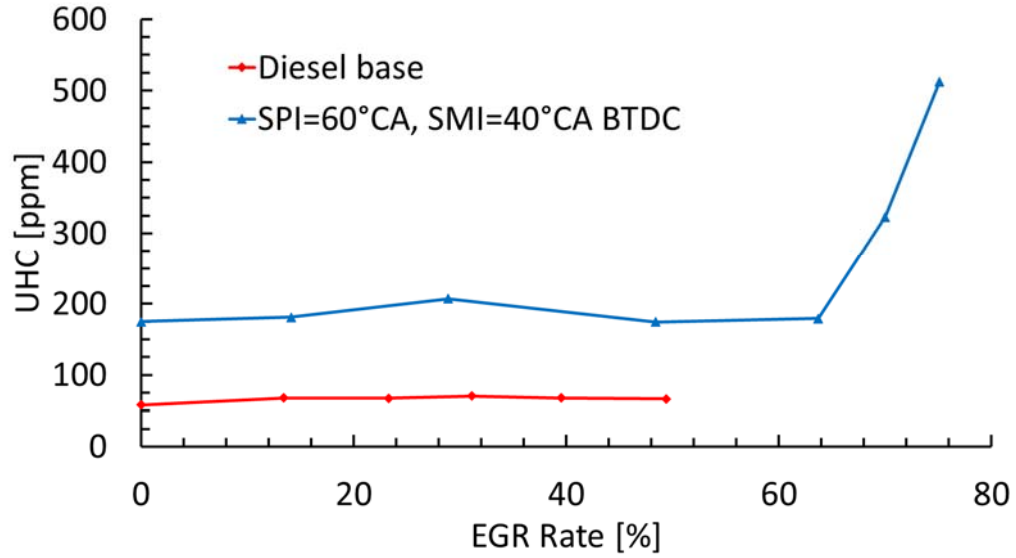


Figure 3.32: Comparison of engine-out UHC emissions according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°C and 40°C BTDC, respectively.

CO emissions of CDC are considerably lower when compared to DIS-PCCI operation. Additionally, these emissions remain stable for all EGR rates examined in the research, as shown in **Figure 3.33**. On the contrary, in DIS-PCCI operation, CO emissions gradual increase with an increase in EGR rate until the 50% EGR rate. Subsequently, for the 65% EGR rate, the CO emissions reach the level of 4000 ppm due to the rapid degradation of combustion.

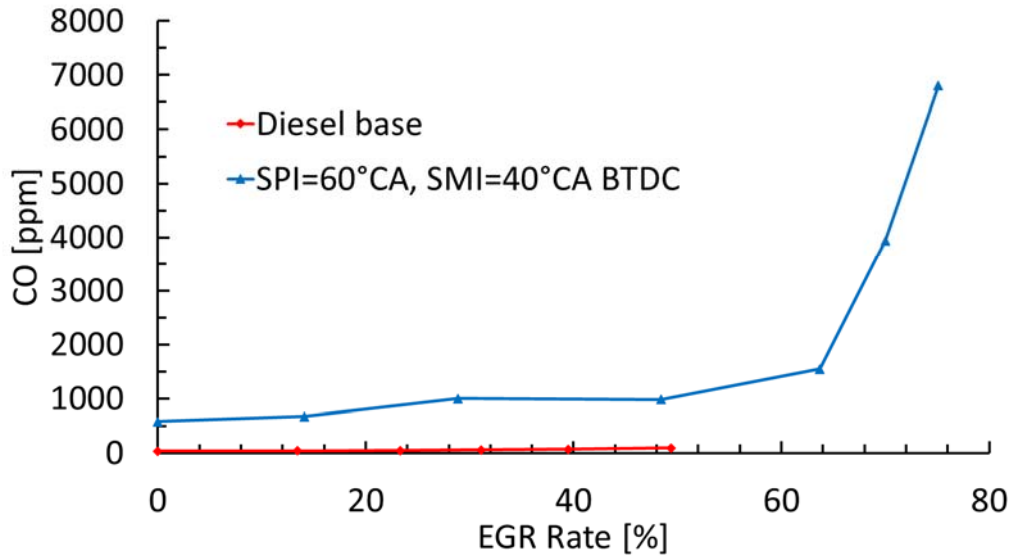


Figure 3.33: Comparison of engine-out CO emissions according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°C A and 40°C A BTDC, respectively.

Figure 3.34 displays the impact of varying EGR rates on the ISFC of CDC and PCCI operations with SPI-SMI pairs of 60°C A and 40°C A.

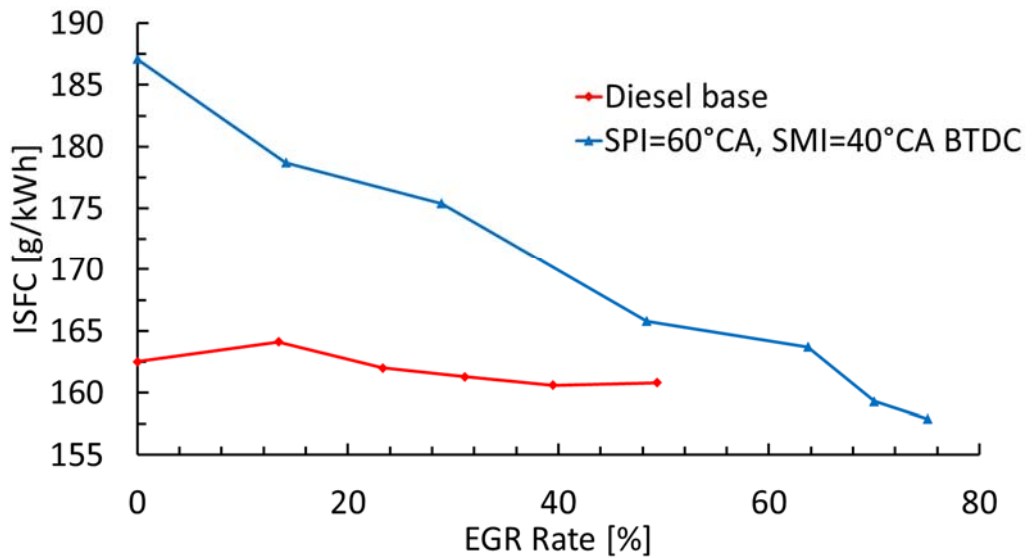


Figure 3.34: Comparison of ISFC according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°C A and 40°C A BTDC, respectively.

Figure 3.35 compares Product of combustion and heat transfer efficiencies (PCHTE) for CDC and PCCI operation with SPI-SMI pair of 60°C A and 40°C A BTDC,

respectively, according to EGR rate. The results indicate that heavy EGR rates over 40% can effectively enhance PCHTE of early DIS-PCCI combustion by up to 10% when compared to CDC, primarily due to the significant improvement in heat transfer efficiency (THE).

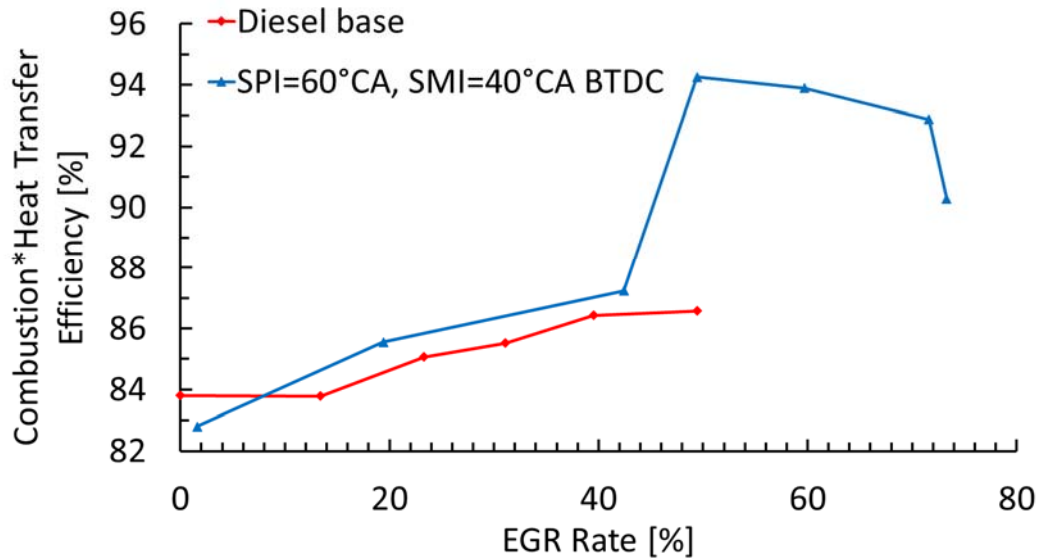


Figure 3.35: Comparison of PCHTEs according to EGR rate for CDC and PCCI operation with SPI-SMI pair of 60°C and 40°C BTDC, respectively.

The PCCI cases exhibit a rise in CCE, increasing from 44.55% to 52.84% as the EGR rate elevates from 0 to 75%. The prolonged ID and lowered HRR, which reduce combustion temperature and wall heat losses, lead to this increase in CCE of PCCI combustion as demonstrated in **Figure 3.36**. MFB50% in PCCI cases ranges from 20.3 to 6.7 °CA BTDC, approaching TDC due to an extended ID and combustion duration, resulting in a lower HRR profile with an increase in EGR rate, as shown in **Figure 3.37**. Therefore, the increase in EGR rate from 0 to 75% causes a decrease in ISFC from 187 g/kWh to 158 g/kWh in PCCI cases, due to reduced heat losses and an increase in net useful work, in accordance with the decrease of the compression work significantly exceeding that of the useful expansion work as seen in **Figure 3.29**. In contrast, for the EGR sweep of CDC, CCE ranges between 51.2% and 51.99%, MFB50% remains constant at 4 °CA BTDC, while ISFC declines from 162 g/kWh to 160.8 g/kWh as the EGR rate increases to 75%.

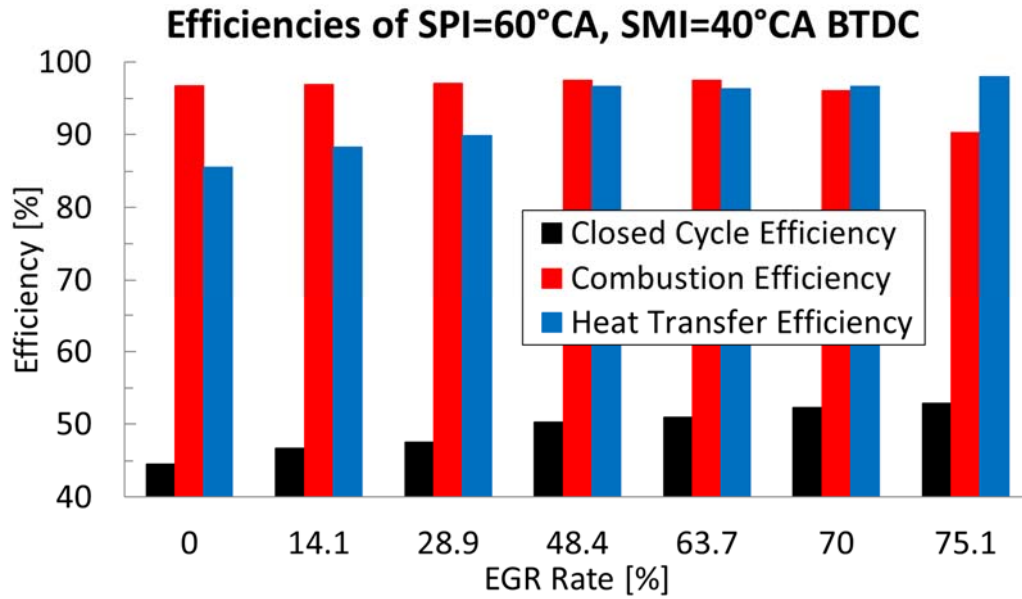


Figure 3.36: CE, HTE and CCE according to EGR rate for DIS-PCCI operation with SPI-SMI of 60°C A and 40°C A BTDC, respectively.

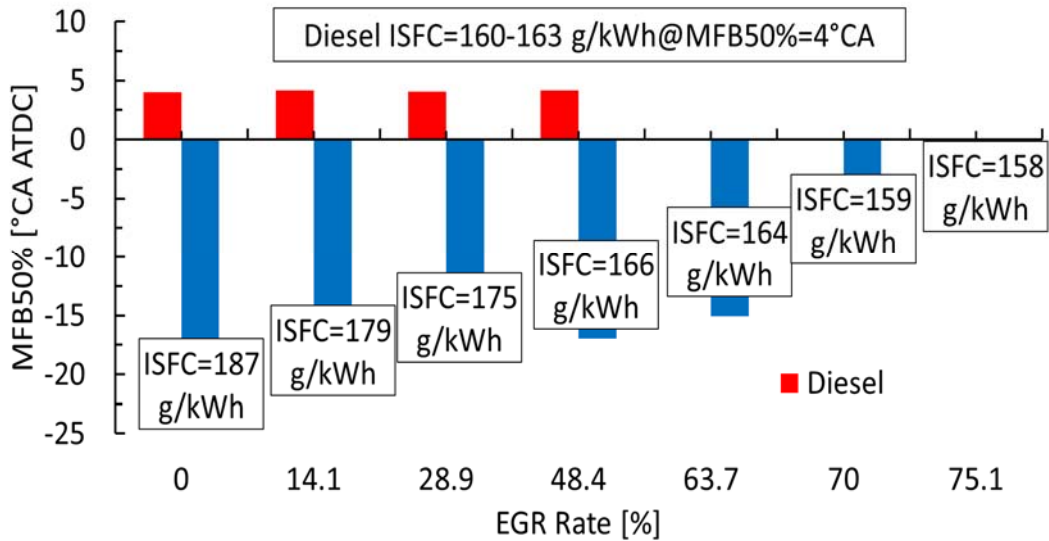


Figure 3.37: Comparison of MFB50% and ISFC according to EGR rate for CDC and DIS-PCCI operation with SPI-SMI pair of 60°C A and 40°C A BTDC, respectively.

The performance of the DIS-PCCI operation was analyzed based on the combustion efficiency, heat transfer efficiency (HTE) and overall closed cycle efficiency (CCE) at different rates of EGR. The results showed in **Figure 3.36** that CE slightly increased from 96.8% to 97.5% as the EGR rate increased from 0% to 60%. However, at EGR rates above 70%, CE decreased rapidly to 90.3% at 75.1% EGR rate due to the

equivalence ratio exceeding unity. HTE increased from 85.6% to 96.7% as the EGR rate increased from 0% to 48.4%. EGR had a significant effect on decreasing combustion temperature and wall heat transfer, particularly at EGR rates above 50%. Despite this, HTE remained above 96% for EGR rates above 50%.

Divergent results can be observed between ISFC and MFB50% for CDC and DIS-PCCI operation with SPI-SMI pair of 60°C_A and 40°C_A BTDC, according to EGR rate in **Figure 3.37**, respectively. Specifically, the ISFC of DIS-PCCI combustion decreases as the EGR rate increases, aligning with MFB%50 approaching to TDC. Nonetheless, DIS-PCCI combustion exhibits higher ISFC than CDC for EGR rates below 68%. Conversely, when the EGR rate is further increased, DIS-PCCI combustion's ISFC is lower than CDC's. For instance, DIS-PCCI combustion can achieve up to 2g/kWh ISFC improvement with a 70% EGR rate. CDC's optimum MFB50% is 4°C_A ATDC. However, DIS-PCCI combustion's ISFC is inferior to CDC's for EGR rates ranging between 68% and 70%, which results in MFB50% between 11.5°C_A and 10°C_A BTDC.

4. COMPUTATIONAL STUDY OF PCCI COMBUSTION

4.1. Theory of Combustion in Engines

In this research, complete IC engine 4 stroke cycle analyses were conducted using 3D CFD simulations carried out with the compressible, reactive, transient flow solver known as CONVERGE [110]. The study delved into the turbulent flow of intake gas feed, spray injection, combustion modelling of chemical kinetics with exhaust emission predictions in a CI SCRE engine model. Fuel sprays are modeled through by using some functions such as probability density functions with including the momentum, transport effects to make an accurate distribution [111], [112], [113]. Reynolds Average Navier Stokes (RANS) equations are used to model turbulence inside the combustion chamber, and renormalization group (RNG) $k-\varepsilon$ turbulence model with the implantation of RNG is used due to the less dissipation rates of eddies and it is more accurate solution for engine applications [114], [115]. Kelvin-Helmholtz Rayleigh-Taylor spray break-up model is used for break-up [116], [117]. Drop-drop collision model specially implemented for hydrocarbon is used for diesel spray droplet collision [118]. vaporization [113], [119], and wall interaction [120], [121].

Reynolds averaged conservation equations for turbulent transport of mass, momentum, thermal energy, and species are presented below. Conservation of mass for compressible flow is given by equation (4.1).

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \quad (4.1)$$

where, x_i is the cartesian coordinate and u_i represents velocity component in the i^{th} direction, ρ is the density, S is source term of diesel spray, and t is the time.

Conservation of momentum for compressible flow in the i^{th} direction is expressed by equation (4.2).

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \quad (4.2)$$

where, stress tensor is given by the equation (4.3).

$$\sigma_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \quad (4.3)$$

In the equations, P represents pressure, S_i is the momentum source due to interaction with the liquid phase, μ is the sum of molecular and turbulent viscosities, and δ_{ij} is the Kronecker delta. Conservation of thermal energy is stated as by the equation (4.4).

$$\begin{aligned} \frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_j e}{\partial x_j} = & -P \frac{\partial u_j}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\frac{K}{c_v} \frac{\partial e}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left[\left(\sum_m h_m \rho D - \sum_m e_m \gamma \frac{K}{c_p} \right) \frac{\partial Y_m}{\partial x_j} \right] \\ & + \dot{Q}^c + \dot{Q}^s \end{aligned} \quad (4.4)$$

where, ρ is density, e is the specific internal energy, K is the sum of molecular and turbulent thermal conductivities, Y_m is the species m mass fraction, h_m is the specific enthalpy of species m , c_p is the specific heat capacity at constant pressure, c_v is the specific heat capacity at constant volume, D is the mass diffusion coefficient, respectively, γ is the ratio of specific heat capacities, and $\dot{Q}^c$ and $\dot{Q}^s$ are energy source terms due to chemical reactions and interaction of turbulent gas flow with spray, respectively.

Conservation of the species can be expressed by the equation (4.5).

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_m}{\partial x_j} \right) + S_m \quad (4.5)$$

where, ρ and u_i are the mixture density and velocity component in i th direction, ρ_m , Y_m and S_m are density, mass fraction and mass generation or destruction rate per unit volume of species m , respectively. Fractional density of a specific species m is given by the equation (4.6).

$$\rho_m = Y_m \rho \quad (4.6)$$

Rapid Distortion RNG approach of k- ε turbulence model is used to derive the turbulence model. The Rapid Distortion RNG k- ε turbulence model is successful to describe the compressed swirling/tumbling flow within a cylinder. The rapid distortion RNG k- ε turbulence model is preferred which is suitable for engine simulations of wall heat distributions where wall are closed to each other. This model is used when turbulent Prandtl number is increased in the boundary layer [115]. The turbulent kinetic energy transport equation is given equation (4.7).

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = -\tau_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial (\mu + \mu_t \sigma_{ij})}{\partial x_j} \frac{\partial k}{\partial x_j} - \rho \varepsilon + \frac{C_s}{1.5} S_s \quad (4.7)$$

where, k is the turbulent kinetic energy, ε is the dissipation of turbulent kinetic energy, τ_{ij} is the Reynolds stress term, Pr_k is the Prandtl number, C_s is a constant and has been suggested 1.5 for diesel sprays, S_s is a spray source term.

Reynolds stress τ_{ij} is given by equation (4.8).

$$\tau_{ij} = -\bar{\rho} \widetilde{u'_i u'_j} = 2\mu_t S_{ij} - \frac{2}{3}\mu_t S_{ij} \left(\rho k + \mu_t \frac{\partial \widetilde{u'_i}}{\partial x_i} \right) \quad (4.8)$$

where the Favre average, $\sim$, is defined for velocity given by equation (4.9).

$$\widetilde{u'_i} \equiv \frac{\overline{\rho u'_i}}{\rho} \quad (4.9)$$

where, k , is given by the equation (4.10).

$$k = \frac{1}{2} \widetilde{u'_i u'_i} \quad (4.10)$$

where the turbulent viscosity, μ_t , is given by given by the equation (4.11).

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (4.11)$$

where C_μ is a model constant, ε is the dissipation rate, S_{ij} is the mean strain rate tensor is given by the equation (4.12).

$$S_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (4.2)$$

The dissipation of turbulent kinetic energy transport equation is given by the equation (4.13).

$$\begin{aligned} \frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho u_i \varepsilon}{\partial x_i} = & \frac{\partial y}{\partial x_j} \left(\frac{\mu + \mu_t}{Pr_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right) + \left(\frac{2}{3} C_{\varepsilon 1} - C_{\varepsilon 3} + \frac{2}{3} C_\mu C_\eta \frac{\partial y}{\partial x} \right) \rho \varepsilon \frac{\partial u_i}{\partial x_i} \\ & + \left((C_{\varepsilon 1} - C_\eta) \frac{\partial u_i}{\partial x_j} \tau_{ij}^* - C_{\varepsilon 2} \rho \varepsilon + C_s S_s \right) \frac{\varepsilon}{k} \end{aligned} \quad (4.13)$$

where S_s is the source term of spray that used to make an energy transfer from droplets to gas phase. The $C_{\varepsilon i}$ terms are model constants that account for compression and expansion. C_η is given by the equation (4.14) and (4.15).

$$C_\eta = \frac{\eta(1 - \eta/\eta_0)}{1 + \beta\eta^3} \quad (4.14)$$

and,

$$\tau_{ij}^* = \tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = 2\mu_t \left(S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad (4.15)$$

Interactions of turbulence with the discrete phase is included by the source term S_s is given by the equation (4.16).

$$S_s = \frac{\sum_p N_p (F'_{drag,i} u'_i)_p}{V} \quad (4.16)$$

where the summation is over all parcels in the cell, N_p is the number of drops in a parcel, V denotes the cell volume, u'_i is the fluctuation component of the velocity of the gas phase velocity, and fluctuating term of the drag force ($F_{drag,i}$) on a drop is given by the equation (4.17).

$$F'_{drag,i} = \frac{F_{drag,i}}{(u_i + u'_i - v_i)} u'_i \quad (4.17)$$

Fuel spray patterns are tracked using a Lagrangian method, whereby blobs of fuel are randomly introduced into the system with a diameter equivalent to that of the nozzle. These blobs move at a speed that is determined by the rate of injection. In the case of DI diesel engines, the temperature of the walls is typically lower than the boiling point of the fuel. As a result, when fuel droplets hit a dry wall, they spread out and form a thin layer of liquid that quickly evaporates depends on their Weber numbers. Some droplets bounce back, some spread out, and some splash back into the chamber. In this study, dynamic behavior of spray droplets are considered, such as, harmonic oscillator system involving a spring, mass, and damper, allows us to approximate the fluctuating drag coefficient of the droplet in motion. [122].

In the analysis of liquid fuel jet primary breakup near injection point, Kelvin-Helmholtz instability mechanism is acted on the droplets generated by liquid blobs.

This research employs a no-time collision (NTC) model used to calculate approximate the quantity of droplet collisions.[123].

The calculation of spray droplet dispersion involves considering the fluctuation of turbulent velocities and the kinetic energy dissipation rates in gas phase related with the effect of turbulent eddies on the droplets. Additionally, O'Rourke droplet collision model is used to include droplet splashing effects into the numerical calculations. This model assumes that each fluctuating velocity component follows a Gaussian distribution [113].

The performance and emissions of a CI diesel engine are heavily impacted by the homogeneity of air fuel vapor mixture (AFVM). Therefore, spray penetration, and distribution of the fuel spray, including atomization, breakup, evaporation mechanism is very crucial. At the end, uniformity of AFVM determines the quality of combustion. Poor atomization, poor uniformity of AFVM, or spray impingement on metal surfaces in the engine can lead to inadequate fuel evaporation rates and mediocre air-fuel vapor mixing. This can increase soot emissions. However, if fuel evaporates too quickly before auto-ignition, NO_x emissions can increase due to fast premixed combustion at high temperatures [124].

There are a multitude of evaporation models available in literature that can effectively compute mass and energy transfer of fuel droplet consisting of a single component and can be utilized in simulations of combustion in DI diesel engines [113], [119], [125], [126], [127].

This research assumes that the temperature within each droplet is uniform and uses two ODEs to determine the changes in temperature and size over time. The equations incorporate Frossling correlations to calculate the rates of heat and mass transfer on the droplet's surface during forced convection [113], [119].

In conclusion, a rebound/slide approach has been integrated to take account of spray impingement on cylinder surfaces [120], [121].

To maintain computational efficiency in CFD simulations is very critical to reduce the computational afford. For this purpose, Adaptive Mesh Refinement (AMR) algorithm is utilized to limit the maximum cell size. In this study, up to 3 million cells are used in the simulations. This algorithm automatically inserts finer cells in areas where the temperature and velocity fields exhibit high gradients, allowing for accurate resolution of flow features away from boundaries. Additionally, excessive refinement near walls is removed to have an optimum computational efficiency to achieve required y^+ level [128]. In this study, the adaptive mesh cell size ranges from 0.25 mm to 4 mm, adjusting based on evolving charge motion and chemical reactions within the cylinder. These mesh settings are suitable for accuracy and resolution of auto-ignition and propagation of reaction zone, while calculating such parameters of spray penetration and flame lift-off length.

4.2. Modeling of Combustion

SAGE chemistry solver is used to solve chemical reactions in the CFD solver [129]. SAGE uses the CVODE solver to solve systems of ordinary differential equations. This solver is part of the SUNDIALS package, which provides a wide range of solvers for nonlinear and differential/algebraic equations [130]. Reaction rates of all species defined in the mechanism are solved by the algorithm inside SAGE chemistry solver for each cell in the CFD mesh. Then species concentration of each cell is updated with the reaction rates taken from SAGE solver. The variables are updated in the transport equations to calculate density, species concentration and temperature values of the

flow field. The successful implementation of SAGE modeling requires detailed or well-defined reduced mechanism for reliable and accurate predictions of combustion. Converge with SAGE solver can solve complex transport equations, enabling accurate predictions of combustion behavior in various combustion regimes, including ignition, premixed, and mixing-controlled combustion.

A series of elementary reactions of chemical reactions can be expressed by equation (4.18) [131].

$$\sum_{a=1}^A v'_{m,r} \chi_m \Leftrightarrow \sum_{a=1}^A v''_{m,r} \chi_m \quad \text{for } l = 1, 2, \dots, L \quad (4.18)$$

where A is the total number of species, $v'_{m,r}$ and $v''_{m,r}$ are the stoichiometric coefficients for the reactants and products, respectively, for species a and reaction l ; L is the total number of reactions; and χ_m is the chemical symbol for species m . The net production rate of species m is given by the equation (4.19).

$$\dot{\omega}_m = \sum_{r=1}^R v_{m,r} q_r \quad \text{for } m = 1, 2, \dots, L \quad (4.19)$$

Coefficients of species are defined in equation (4.20).

$$v_{m,r} = v''_{m,r} - v'_{m,r} \quad (4.20)$$

The rate-of-progress parameter for q_r the r^{th} reaction is given by the equation (4.21).

$$q_r = k_{fr} \prod_{m=1}^M [X_m]^{v'_{m,r}} - k_{rr} \prod_{m=1}^M [X_m]^{v''_{m,r}} \quad (4.21)$$

In Equation 4.19, X_m is the molar concentration of species m , and k_{fr} and k_{rr} are the forward and reverse rate coefficients for reaction r . Forward reaction rate coefficient is expressed in equation (4.22).

$$k_{fr} = A_r T^{b_r} e^{(-E_r/R_u T)} \quad (4.22)$$

where A_r is the pre-exponential factor, br is the temperature exponent, E_r is the activation energy, and R_u is the universal gas constant. The equation governing mass can for a given species can be expressed by the equation (4.23).

$$\frac{d[X_m]}{dt} = \dot{\omega}_m \quad (4.23)$$

The governing equation to calculate change of temperature in time is given by equation (4.24).

$$\frac{dT}{dt} = \frac{V \frac{dP}{dt} - \sum_m (\bar{h}_m \dot{\omega}_m)}{\sum_m ([X_m] \bar{c}_{p,m})} \quad (4.24)$$

Where P is pressure, $\dot{\omega}_m$ is determined by equation (4.21), and $\bar{h}_m$ and $\bar{c}_{p,m}$ are the molar specific enthalpy.

In this study, n-heptane (n-C₇H₁₆) is chosen as a surrogate fuel of diesel. Therefore, chemical mechanism of n-heptane is used to model the premixed and diffusion-controlled combustion which includes all the forms of low temperature and conventional diesel combustion [132]. N-heptane combustion characteristics such as cetane number, auto-ignition temperature, ignition delay is similar to diesel fuel. On the other hand, thermophysical properties of n-heptane is differ from diesel fuel. To perform a accurate simulation, thermophysical characteristics of diesel fuel can be well defined to predict spray penetration rate, spray break-up, flame-liftoff length, droplet dispersion and AFVM homogeneity. Therefore, thermophysical properties of tetradecane (C₁₄H₃₀) of boiling point, vapor pressure, viscosity, thermal conductivity, surface tensions is preferred to use in the simulation.

Nevertheless, since n-heptane has a higher net calorific value than regular diesel fuel, a correction factor is used to equalize the same chemical heat rejection. To model the combustion kinetics, a reduced mechanism consisting of 42 species and 168 elementary reactions of n-heptane is used in this thesis [133]. The reaction mechanisms the is studied in this report is shown in **Appendix-A**.

In the diesel combustion simulations, a validated methodology involves a reduced n-heptane integration of Engine Combustion Models of Detailed In-Cylinder Optical

Diagnostics Data for a Heavy mechanism and employing direct time integration without a sub-grid turbulence-chemistry interaction model. This approach has demonstrated accuracy in predicting crucial engine parameters and in-cylinder phenomena, such as ignition delay, in-cylinder pressure, and apparent HRR histories, as well as the location of cool and hot flame ignition and second-stage combustion sites, and the distribution of soot and OH. This method has proven effective in both low and high-temperature combustion scenarios, regardless of the timing or quantity of fuel injections in compression ignition engines. This has been tested and validated on the KIVA-CHEMKIN platform [134], [135] .

The extended Zel'dovich mechanism of three fundamental reactions involving seven species, has been employed to calculate NO emissions [23]. To convert NO into NO_x, a mass scaling factor of 1.533 has been utilized in the process. In addition, the De Soete model was used in computational fluid dynamics simulations to calculate the small contribution (less than 5%) of prompt NO_x. Prompt NO_x reactions can only be functional on very low temperatures, near stoichiometric and rich flames, under the presence of hydrocarbon radical generation that it is only be generated in the early phase of diesel combustion [136].

Hiroyasu- Nagle and Strickland-Constable (NSC) model is used to calculate soot emission that Hiroyasu is responsible from the soot generation and NSC is deals with soot oxidation [137], [138].

In this study, a full geometric model of SCRE engine is used. The model consists of all the parts used in the engine. Combustion related non-moving parts of cylinder head, liner, intake charge ports and manifold, and exhaust ports, moving parts of piston and valve are fully implemented into the model. Engine geometry is illustrated in **Figure 4.1**.

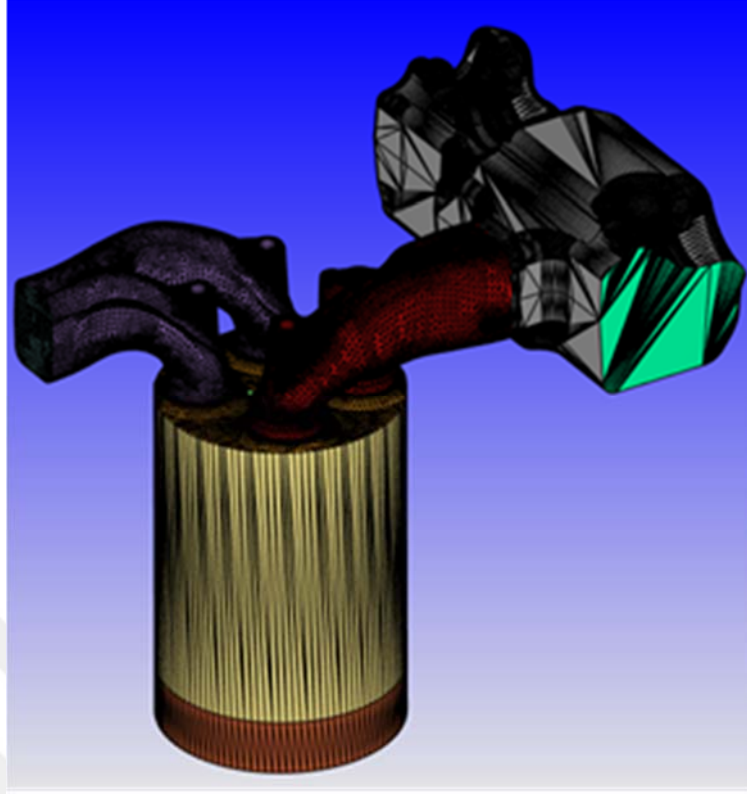


Figure 4.1: Engine geometry used in the simulations.

Simulations begin at the stage of a complete cycle to prevent any disturbances of previous cycles which start 168°CA ATDC. and run 720° of crankshaft rotation to ensure accurate calculation of flow during each stroke. Cycle-averaged wall temperature distributions are mapped for all combustion chamber surfaces generated by conjugate heat transfer calculation [139]. Average values of wall temperature values and boundary conditions of the simulation is given in **Table 4.1**.

Table 4.1: Average temperature values of wall boundaries and intake boundary conditions used in the simulations.

Absolute inlet manifold pressure [bar]	1.36
Air inlet temperature [K]	298
Average piston temperature [K]	543
Average liner temperature [K]	398
Average cylinder head temperature [K]	521

Operating conditions and important engine parameters of the simulations are shown in **Table 4.2**.

Table 4.2: Operating conditions and important engine parameters.

Parameter	Unit	Value
Engine Speed	rpm	1100
Intake pressure	bar abs.	1.425
Injected fuel mass	mg/stroke	39
Air to fuel ratio	-	71:1
Injection pressure	bar	800
Spray inclusion angle	degree	146
Injector nozzle diameter	μm	180
Number of nozzles	-	8

4.3. Validation of the Studies

In this section, 3D CFD simulation results are validated by the test engine measurements described in the previous section. 3D CFD combustion simulations are compared with test data based on engine measurements. Validation studies are performed with single main injection event, both on conventional late start of injection strategy of including premixed and diffusion-controlled combustion, and a very injection of PCCI strategy.

Pressure and apparent heat release histories of part load operation of CDC and PCCI combustion simulations are compared with engine tests for advanced and late injection cases of 10°CA & 50°CA BTDC in **Figure 4.2** and **Figure 4.3**, respectively.

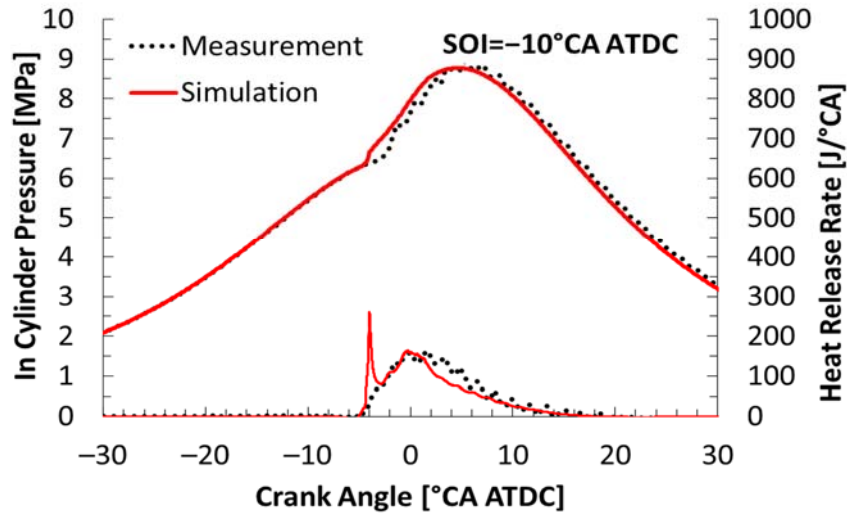


Figure 4.2: Validation of measured and predicted in-cylinder pressure and apparent HRR histories of SOI=-10 °CA ATDC.

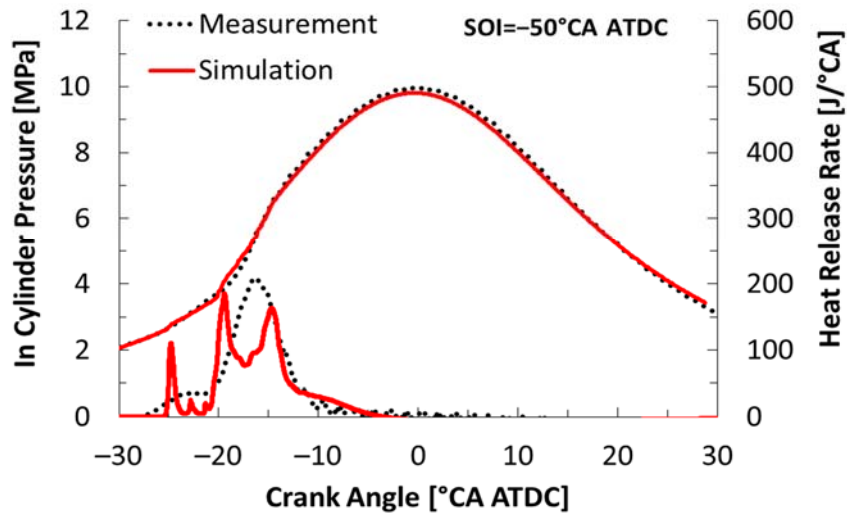


Figure 4.3: Validation of measured and predicted in-cylinder pressure and apparent HRR histories of SOI=-50 °CA ATDC.

In the retarded injection strategy of the conventional diesel combustion, self-ignition of rich fuel-vapor-air mixture preparation occurs near to the fuel spray tip with an ignition delay $\sim 4.5^\circ\text{CA}$. Such an occurrence triggers the pre-mixed combustion at a relatively lower gas temperature conditions, proceed with sudden increase heat release rate and OH production, thereby instigating the production of PAH and CO, as represented in Figure 4.2.

In the downstream of combustion, soot production starts in the relatively higher temperature region of oxygen lean zone inside the diffusion flame. After premixed combustion, oxidation of intermediate species of chemical kinetics takes the role into the CO_2 , H_2O and NO_x in the diffusion-constrained, high-temperature environment. It is noted that, an accurate prediction of in-cylinder pressure and apparent HRR of diffusion-controlled phase of diesel combustion is achieved. But maximum value of the apparent HRR of the premixed zone of the simulation cannot be seen in the measurement data results due to filtering settings and sample rate selection.

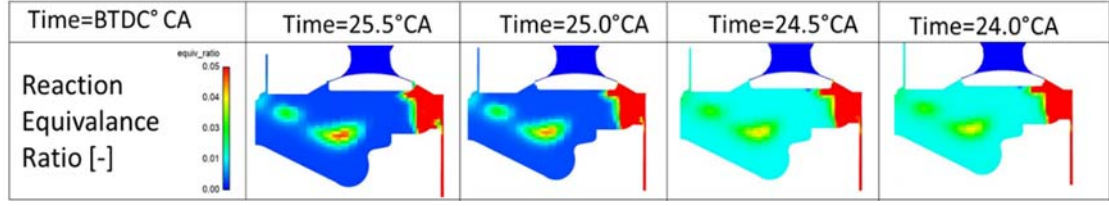
CFD simulation of PCCI combustion with a start of injection of 50°CA BTDC reveals a substantial delay of $\sim 25^\circ\text{CA}$ because of injection into the relatively low temperature conditions. Such a delay precipitates an inhomogeneous AFVM, which triggers 5 local peaks of apparent heat release rate generation. These sudden ignite and quench events are associated fuel concentration and gas temperature ranges in AFVM.

The advanced single injection strategy exhibits a rapid three premixed lean combustion zones in very lean AFVM of $\sim$ reaction equivalence ratio (RER)=0.04 under the exhaust valves which is relatively high temperature in the combustion chamber. These cool flames are quickly quenched due to consumption of the available AFVM, the coolant effect of the evaporation through the liquid fuel, high amount of the unburnt gas all around the cool flame zone and lower temperature values of the cylinder walls. These factors results temperature reduction around these flame initiation zone and quenching occurs.

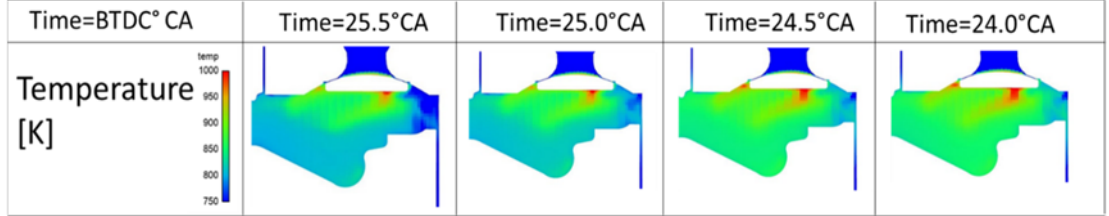
Flame initiation and quenching progress is repeated where AFVM and temperature is sufficient to start ignition. In the later phase of the combustion process, two major combustion events occur on the wide area of the combustion chamber without any flame extinguishes that AFVM and the temperature levels are higher due to the elevated fuel evaporation rate and piston position of compression stroke. Combustion gradually completed when fuel is totally consumed before top dead center. Consequently, the AFVM starts to ignite starting from 700-750 K reaches above 1000 K on the premixed combustion of cool flames, and ultimately peaks above 2800 K during main combustion event until fuel is consumed proximate to TDC.

Figure 4.4 presents distribution of reaction equivalence ratio, gas temperature, and OH concentration at 25.5°, 25.0°, 24.5°-24.0°CA BTDC of SOI=50 °CA BTDC. These figures present the position of first auto-ignition event due to advanced start of injection strategy. The contour plots are displayed in a plane that traverses the combustion chamber and liquid spray center with the OH concentration of iso-surface of 1×10^{-7} shown in the overhead of the piston. Preceding the first auto-ignition, fuel vapor congregates in proximity to the engine metal surfaces and generates spots inside the piston crown which has limited momentum of spray droplets.

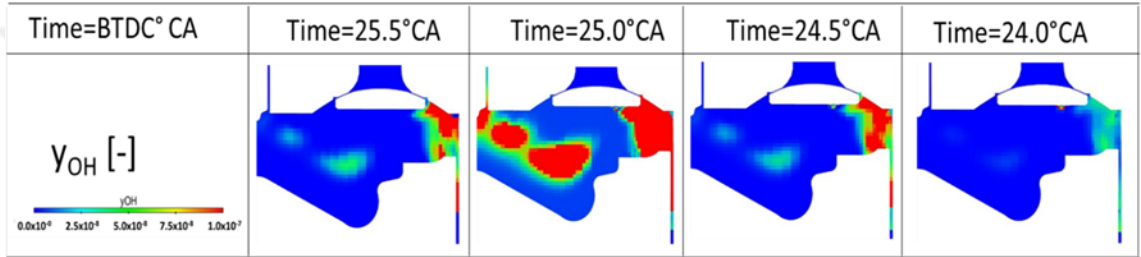
Cool flames are occurring during the auto-ignition of the lean AFVM regions with temperatures exceeding 850-900 K are generated at these spots in the crevice region, with an equivalence ratio of 0.05-0.2. Local rapid combustion of cool flames occurs above 1000-1200K under the exhaust valve with a reaction equivalence ratio above 0.05. However, rapidly extinguish occurs due to lower AFVM. These auto-ignition zones and temperature increase in combustion chamber is seen in **Figure 4.4b**. Production and consumption of OH-radicals inside the engine and its concentration on the given piston positions are illustrated in **Figure 4.4c**. Finally, distribution OH concentration of 1×10^{-7} in the given piston position of first auto-ignition is seen in **Figure 4.4d**.



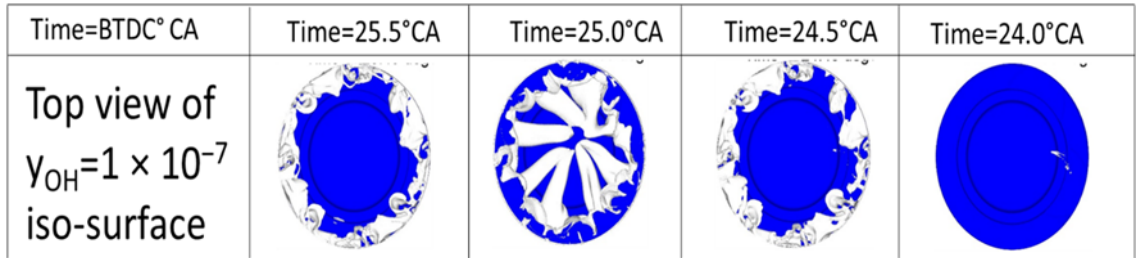
(a)



(b)



(c)



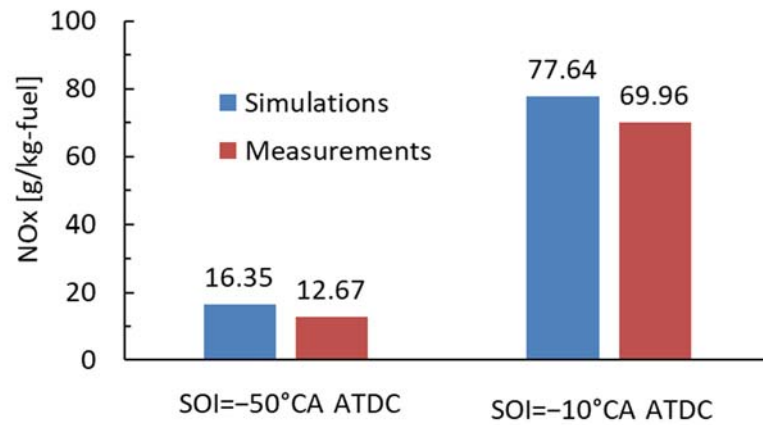
(d)

Figure 4.4: Cut views of (a) reaction equivalence ratio; (b) temperature; (c) OH concentration; (d) propagation of OH concentration at start of initial auto-ignition at 25.5°, 25.0°, 24.5°-24.0°CA BTDC of SOI=50 °CA BTDC.

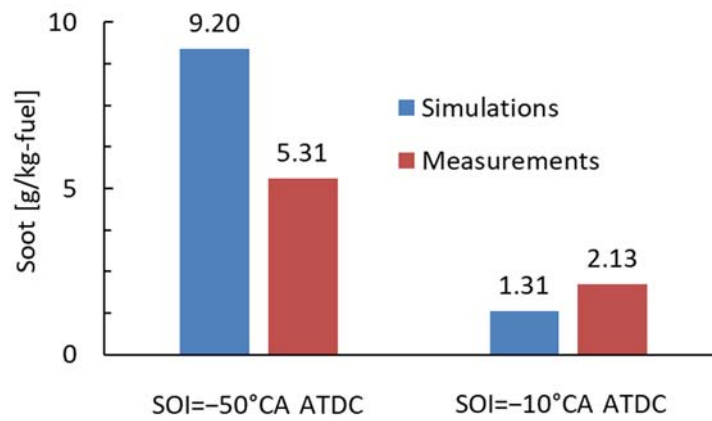
Differences between simulation results and measurement of NO_x , soot, and CO emissions are presented in **Figure 4.5** for both injection timings. While NO_x and CO emission of CFD results are aligned with test results, significant disparities are observed in calculated and measured soot emissions, especially in PCCI combustion. The Hiroyasu with Nagle Strickland-Constable Oxidation soot model predicts soot emissions two times higher in advanced injection case. It is also advised to tune the model parameters including the pre-exponent factor and scaling factor to have a better

soot model correlation. Soot production and oxidation rates should be tuned to have an accurate model of advanced and retarded combustion cases. Additionally, the formation of much smaller child droplets due to increased surface area resulting from the splashing of liquid fuel droplets hits directly into the wall enhances evaporation and fuel-air mixing rates, resulting in decreased soot-formation rates [140]. However, droplet model used in this study does not account for the splashing of impinging droplets.

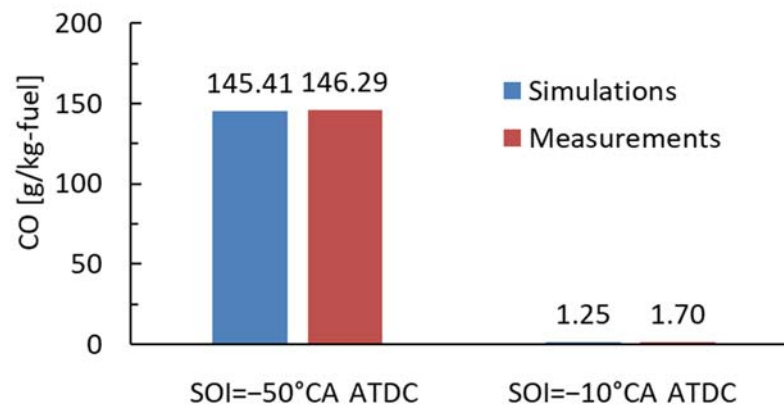




(a)



(b)



(c)

Figure 4.5: Validation of simulated and measured exhaust (a) NO_x; (b) soot; (c) CO emissions.

In the case of the CDC, interestingly, there is minimal difference between the simulated and dyno test soot emissions, with an SOI of 10 °CA BTDC. This is because rich-premixed phase of combustion begins prior to the injector nozzle exit impinging on the edge of the piston crown, at a temperature of 750 K. As a result, the liquid form spray is evaporated during penetration and mixed with air successfully in the combustion chamber. A well AFVM is obtained into piston bowl and above the edge of piston in the diffusion combustion stage.

4.4. Effect of Spray Injection Timing on Combustion, Emission and Performance

To achieve optimal combustion in a low-load, low-speed DI diesel engine without using EGR, injection timing plays a crucial role. Early start of injection timing results in premixed combustion with multiple short AHRR peaks, followed by main combustion events that release a significant amount of heat. When injection timing is very advanced, liquid phase of fuel has enough timeline to evaporate and achieve a better AFVM until start of ignition, resulting in well mixed low temperature combustion and reduced NO_x emissions [141]. However, very early start of injection can lead incomplete evaporation, limited breakup and long spray penetration of low temperature conditions inside the cylinder and resulted to wall wetting. Due to lower temperature combustion, incomplete combustion occurs. Extremely low combustion temperature generates cool flames and hydrocarbon oxidation cannot be achieved. Spray wall of fuel rich zones triggers soot formation, and it is resulted with a reduction of combustion efficiency. Late injection timing results a better spray evaporation in the combustion chamber during diffusion-controlled combustion. Combustion takes place in a high pressure, richer AFVM and elevated gas temperature, leading to increased NO_x emissions.

In this part of the study, 3D CFD simulations are performed to investigate the effect of start of injection. In-cylinder pressure, apparent HRR, combustion efficiency; NO_x, soot, and CO formation is investigated in the engine model. The results of SOI=-70 °CA, -50 °CA, -30 °CA, -20 °CA and -10 °CA ATDC are presented in **Figure 4.6** and **Figure 4.7**. It is observed that the maximum two peak firing pressure was achieved with an SOI=-30 °CA and SOI=-20 °CA ATDC.

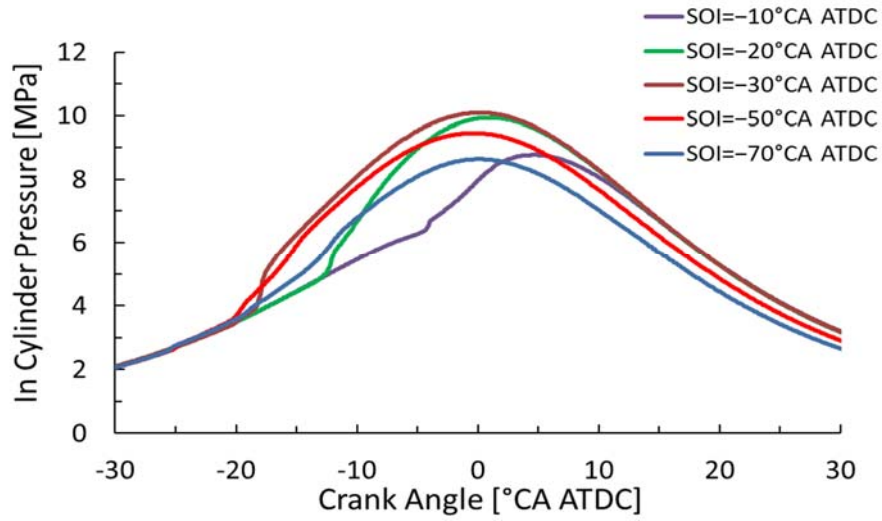


Figure 4.6: In-cylinder pressure histories of various start of injection values.

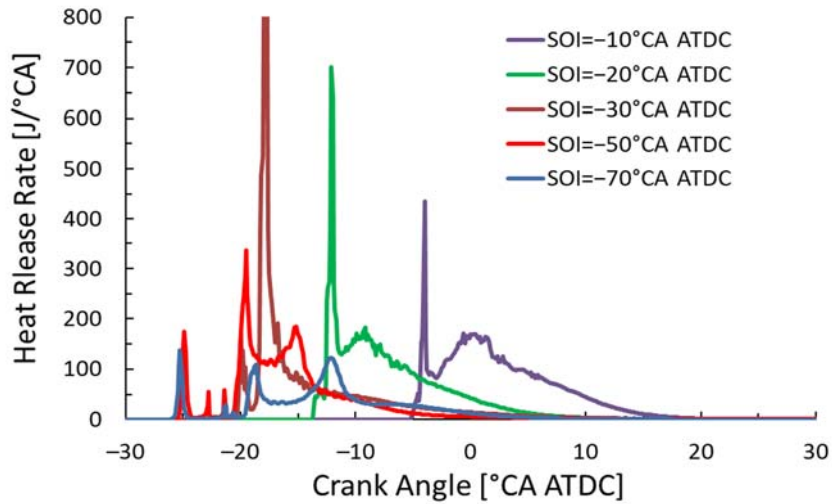


Figure 4.7: Apparent HRR histories of various start of injection values.

In cases where early start of injection of $\text{SOI}=30^\circ\text{CA}$, $\text{SOI}=50^\circ\text{CA}$, and $\text{SOI}=70^\circ\text{CA}$ BTDC, multiple local peak values can be observed in the apparent HRR histories. This is because of the local auto-ignition of low temperature region of lean combustion and formed of cool flames. However, these cool flames are arisen and quenched very rapidly. Then, high temperature combustion at lean conditions due to long ignition delay occurs when the gas temperature reaches above a critical temperature. Although main combustion events are limited to a small zone in $\text{SOI}=70^\circ\text{CA}$ BTDC, flame propagation is covering the volume inside the piston crown and gradual increase in apparent HRR on retarded combustion cases, starting from $\text{SOI}=50^\circ\text{CA}$ BTDC.

In the cases of $\text{SOI}=20^\circ\text{CA}$ or $\text{SOI}=10^\circ\text{CA}$ BTDC, conventional diesel combustion is observed. In the early phase of the injection period, initial AFVM zone starts an auto-ignition in the premixed region. AFVM mixing is formed during ignition delay of the combustion. Combustion of premixed region suddenly releases chemical energy by the high temperature chemical kinetics. This phase of combustion is characterized by a significant spike in the apparent HRR suddenly. Following this, combustion continues with diffusion-controlled and chemical reactions are controlled by AFVM progress. In this step, apparent HRR gradually increases within the effects of combustion temperature to a maximum value and starts to decrease with end of injection. Then apparent heat release decreases due to consumption of fuel vapor and completion of combustion. According to the simulation results, $\text{SOI}=30^\circ\text{CA}$ B TDC generates maximum apparent HRR in the premixed phase of combustion.

In cases where fuel is injected at $\text{SOI}=30^\circ\text{CA}$, $\text{SOI}=50^\circ\text{CA}$, and $\text{SOI}=70^\circ\text{CA}$ BTDC, it is observed when the start of injection is advanced, both peak apparent HRR and the combustion duration of premixed phase decrease. This is because ignition delay of chemical kinetics that can be required due to lower in-cylinder temperature levels, insufficient evaporation rates to combine a better AFVM.

In cases where fuel injection is delayed (late-injection strategy) with a $\text{SOI}=20^\circ\text{CA}$ and $\text{SOI}=10^\circ\text{CA}$ BTDC, a short ignition delay is obtained. Therefore, a decrease in spray break-up, evaporation and AFVM period of premixed combustion results with a small apparent HRR peak. CFD simulations show that, retarded combustion strategies is effective due to higher pressure and temperature values of being in the end of the compression stroke to limit premixed combustion compared to advanced injection cases.

In **Figure 4.8**, SOI_{Ign} of various start of injection strategies are presented. SOI_{Ign} is not highly sensitive to SOI in very advanced injection cases. But a small reduction can be seen in SOI_{Ign} when SOI is retarded. On the other hand, $\text{SOI}=70^\circ\text{CA}$ and $\text{SOI}=50^\circ\text{CA}$ BTDC, ignition starts about 25.5°CA BTDC, On the other hand, SOI_{Ign} is directly effected by SOI timing in late injection events.

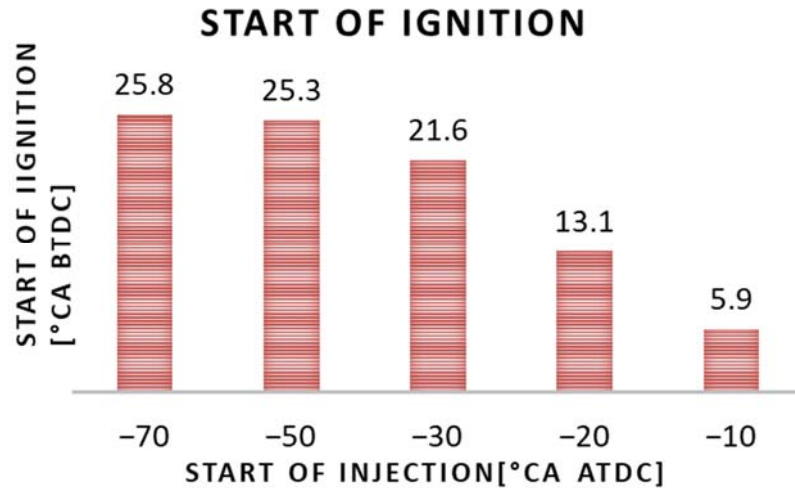


Figure 4.8: SOIgn timings in various SOI.

Figure 4.9 shows the ignition delay corresponding to SOI of advanced and retarded combustion scenarios. However, advanced injections cases of SOI=70°CA and SOI=50°CA BTDC, longer ignition delay is obtained due to low in-cylinder temperature during injection. In contrast, retarded injection cases of SOI=30°CA, SOI=20°CA, and SOI=10°CA ATDC exhibit a short ignition delay when the injection timing is retarded. In these cases, injection is performing at high temperature due to timing of the end of the compression stroke. Retarded injection strategy is characterized by a gradual increase in AHRR during the diffusion-controlled main combustion phase, preceded by a short-lived, high AHRR premixed combustion phase immediately after auto-ignition.

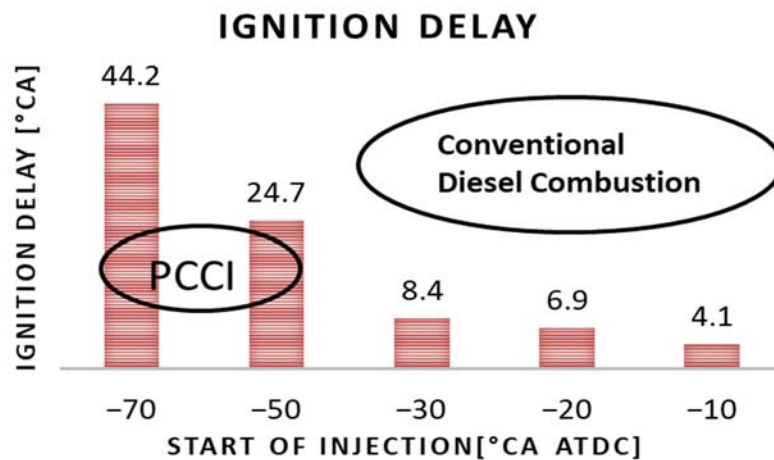


Figure 4.9: Ignition delay in various SOI.

Figure 4.10 shows how NO_x emissions change during compression and expansion strokes as the temperature changes. When fuel is injected early, there is almost no NO_x emissions because of the chemical kinetics in low temperature combustion. However, in the retarded injection, NO_x production is increased because combustion is occurred in high temperature and locally rich under diffusion-controlled combustion. As the timing of fuel injection is advanced, the amount of NO_x emissions gradually increases because of the increase in maximum value of apparent HRR and the combustion duration in the premixed combustion phase. At an $\text{SOI}=30^\circ\text{CA BTDC}$, the temperature level of the premixed combustion sectors reaches its maximum value. If the fuel is injected advanced more than 30°CA BTDC , peak value of the apparent HRR decreases significantly.

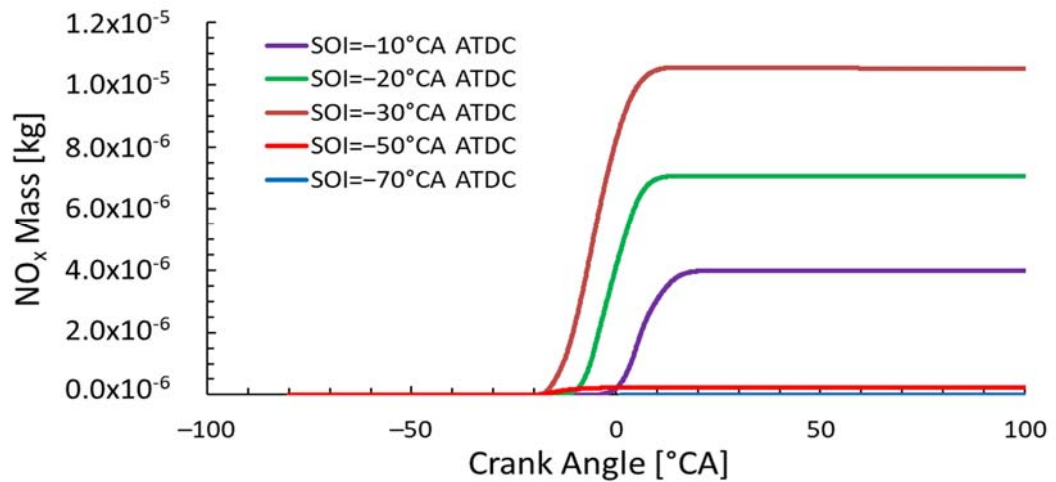


Figure 4.10: Evolution of NO_x formation histories of various SOI.

Figure 4.11 displays how the timing of SOI effects the formation and oxidation of soot on the timeline of the compression and power strokes. When SOI is delayed, soot formation rate is increases but the duration decreases. In PCCI combustion, the formation period of soot is longer than conventional diesel combustion. In the fuel impingement zones of PCCI combustion, due to insufficient oxygen concentration, reaction rate of the combustion, temperature levels and as a result, PAH formation mechanism are limited. However, in higher temperature combustion, inside the diffusion flame due to higher temperature above 1600K environment and low oxygen

concentration, soot precursors and PAH can easily be formed and growth easily to generate soot emissions. However, when SOI is retarded, high temperature of the burnt gas with the help of the oxygen concentration outside the flame, soot oxidation rate increases rapidly. Accumulated soot is consumed in very fast in high temperature combustion. In very advanced injection, the main factor of soot generation is spray to cylinder interaction. Although soot production is smaller than the conventional combustion, soot oxidation is restrained by temperature values of low temperature combustion and cooling effect due to piston movement in the expansion stroke [142]. In diffusion-controlled combustion, huge amount of soot production is observed inside the diffusion flame core in the fuel rich zone. In the combustion event, After the peak of soot mass is reached, oxidation begins, dramatically reducing soot concentration with the help of increased temperature of the flame and gas motion of expansion that transfers the oxygen with soot to allow oxidation mechanism [18], [23], [143].

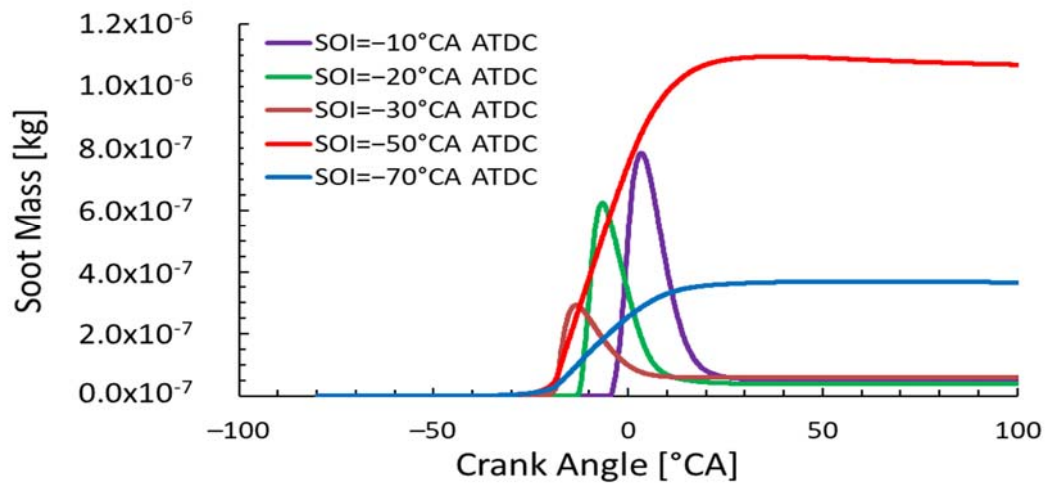


Figure 4.11: Evolution of soot mass histories of various SOI.

Figure 4.12 illustrates the impact of SOI on CO mass histories in the combustion.

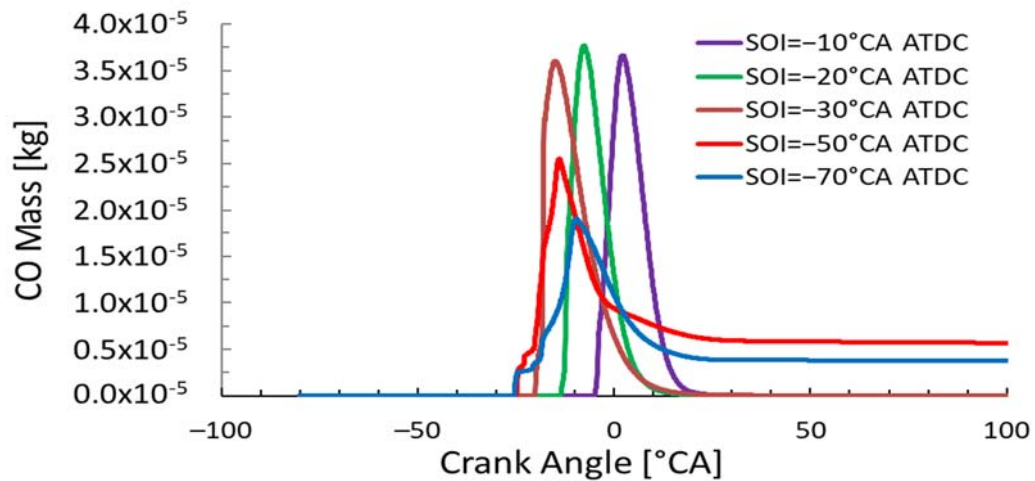


Figure 4.12: Evolution of CO mass histories of various SOI.

It has been observed that formation and consumption levels of CO is significantly higher in retarded injection cases compared to advanced injection cases. This is because of the high combustion temperature levels and complete combustion of the retarded combustion cases. As a result, very low CO is emitted from the engine. Exhaust emissions of various injection strategies have been listed in

Table 4.3.

Table 4.3: Engine-out emissions.

SOI [°CA BTDC]	70	50	30	20	10
NO _x [ppm]	4.0	54.8	3533.3	2368.6	1336.7
Soot [ppm]	147.8	206.8	20.5	13.6	17.1
CO [ppm]	134.3	935.0	22.4	12.6	16.4

Figure 4.13 shows the variations in combustion efficiency and indicated mean effective pressure of various start of injection timings. Advanced injection results a reduction in combustion efficiency and indicated mean effective pressure levels. Spray wall interaction with low temperature of in-cylinder gas effects the combustion temperature and CO and UHC are not totally converted to CO₂. This can see in the calculation of chemic energy release and reduction on combustion efficiency and indicated mean effective pressure due to incomplete combustion. On the other hand, retarded injection timing improves the spray droplets of break-up and evaporation and also combustion occurs on high temperature conditions, resulting in sprays directly

entering the piston crown without impinging on the cylinder liner. Fast evaporation of spray droplets can easily mix with unburnt gas, leading to a richer AFVM in the premixed combustion. Intermediate species and CO can easily be oxidized in high-temperature combustion. Retarded cases of SOI=10 °CA BTDC yields highest combustion efficiency and indicated mean effective pressure.

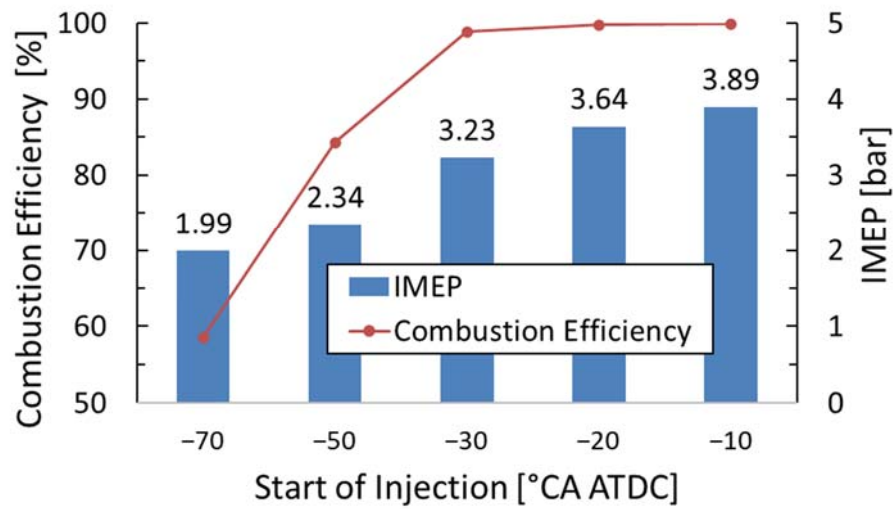
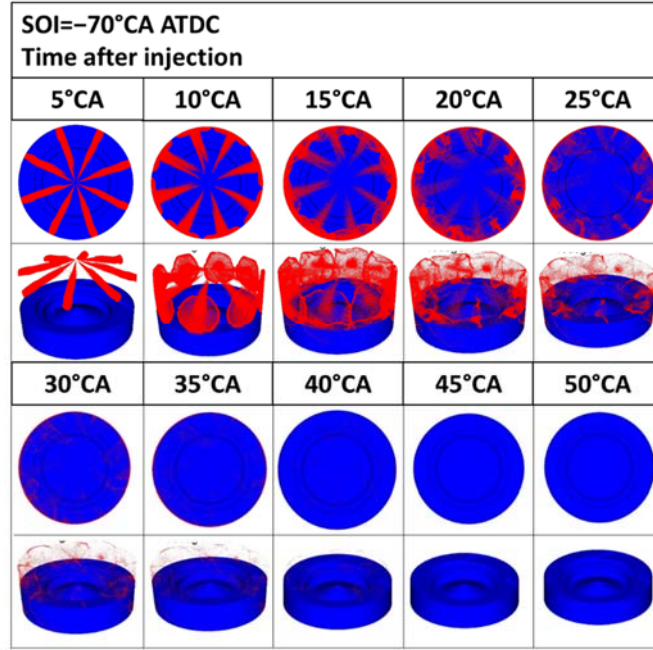
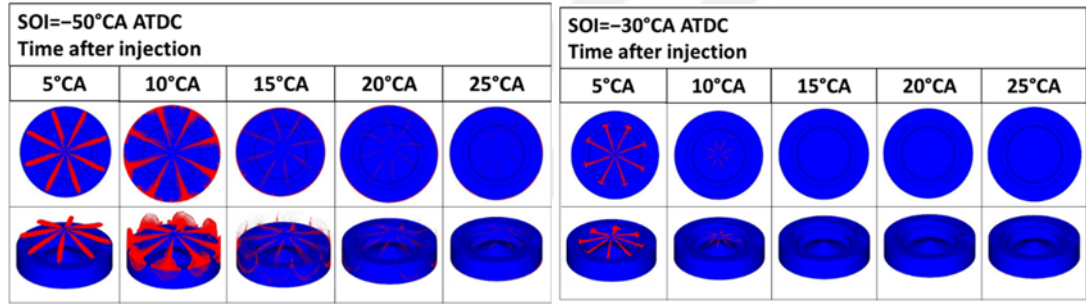


Figure 4.13: CE and IMEP in various SOI.

Figure 4.14 illustrates the progression of sprays in both top and oblique side views after 5,10,15,20,25°CA of SOI=70°CA, 50°CA, 30°CA, 20°CA, 10°CA BTDC.

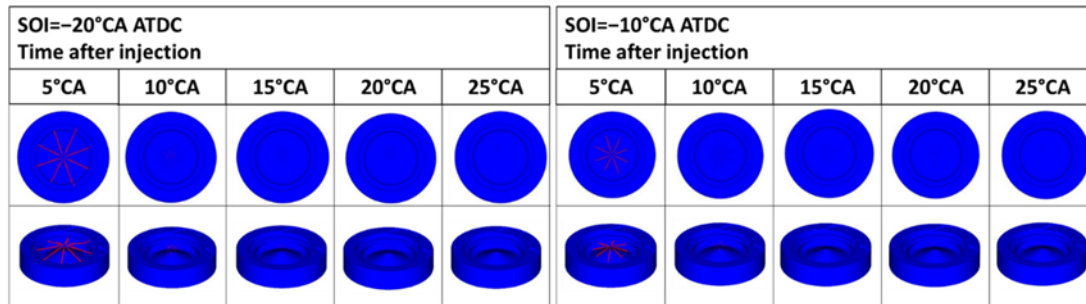


(a)



(b)

(c)



(d)

(e)

Figure 4.14: Top and oblique side views of liquid spray visualization after 5,10,15,20,25°CA of start of injection timings. (a) SOI=70°CA BTDC; (b) SOI= 50°CA BTDC; (c) SOI=30 °CA BTDC; (d) SOI=20°CA BTDC; (e) SOI=10°CA BTDC.

Figure 4.15 presents the effects of SOI on liquid spray mass content inside the cylinder at different °CA ATDC. When SOI is set at 70°CA and 50°CA BTDC, liquid phase of the fuel is totally converted to gas phase when the piston is positioned up to -20°CA

ATDC. In these instances, it takes 48 °CA and 28 °CA for a total evaporation of the fuel, respectively. Conversely, for delayed injection timings, such as SOI=30°CA, SOI=20°CA, and SOI=10 °CA BTDC, the period of complete evaporation is below 10°CA including injection.

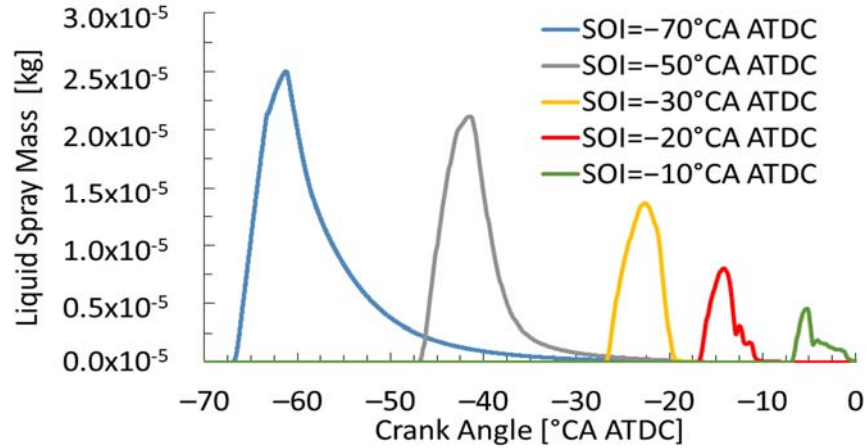


Figure 4.15: Liquid spray mass content of various SOI inside the cylinder at different °CA ATDC.

Figure 4.16 illustrates the spray tip penetration length (STPL) in the radial direction at various SOI timings. The results show that early injection profiles exhibit higher STPLs compared to retarded injection events due to insufficient pressure and temperature levels of the combustion chamber. Specifically, for advanced injection of SOI=70°CA and SOI=50°CA BTDC, liquid form of the spray splash on the walls between 4.0 and 5.0°CA after injection, respectively. In advanced injection of SOI=70°CA BTDC, liquid spray droplets hit the cylinder liner and rebound back into the combustion chamber. Some of the droplets are directed into the crevice volume. Most of the droplets are rotated with the effect of the swirl motion and interact with the neighbor droplets of clockwise direction. Huge amount of the liquid films evaporated between the edge of the piston and cylinder liner before the start of combustion around 26°CA BTDC. In advanced injection event of SOI=50°CA BTDC, fuel spray is directly penetrating into the crevice zone and some of the fuel is splashed from entrance region of crevice volume and evaporates in this region and most of the fuel is evaporated before ignition starts around 25°CA BTDC.

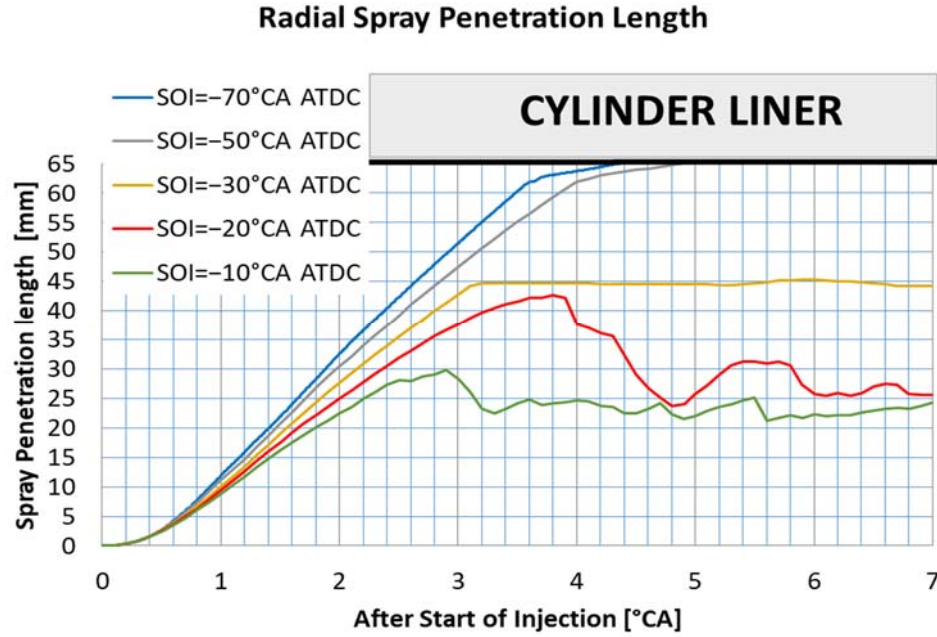


Figure 4.16: STPL histories of spray penetration from the spray center of various SOI.

In retarded injection cases of SOI=30°CA, 20°CA, and SOI=10°CA BTDC, the fuel spray does not impinge on combustion chamber walls. In retarded injection events, there is a sudden drop in STPL after start of ignition. This is because as the gas temperature increases during combustion, the fuel droplets evaporate more quickly compared to spray penetration. The retarded injection events result a complete evaporation of the piston bowl's sprays after around 10°CA due to the elevated temperature and pressure conditions.

RER describes the actual evaporated fuel inside the combustion chamber to figure out the formation of AFVM and richness of the surrounding volume different combustion chamber zones such as liner, head, piston crown, squish and crevice volume. **Figure 4.17** presents the RER histories of SOI=70°CA, 50°CA, 30°CA, 20°CA, 10°CA BTDC timings.

In advanced injection case of SOI=70°CA and SOI=50°CA BTDC, spray interaction with wall and crevice volume results excessive fuel accumulation that results of heavy UHC maintenance in the exhaust emissions. RER distribution of advanced injection events are compatible with the findings of CFD simulations that were validated by Planar Laser-Induced Fluorescence (PLIF) techniques [144].

In contrast, retarding injection event can result in improved fuel-air mixing, thereby avoiding wall impingement. In $\text{SOI}=10^\circ\text{CA}$ BTDC event, the fuel vapor jet separated by the stepped lip geometry of the piston into two streams. The lower stream goes towards to piston crown and mix with fresh air. Th upper stream is directed into the squish region. Therefore, a homogeneous and uniform AFVM can be accomplished.

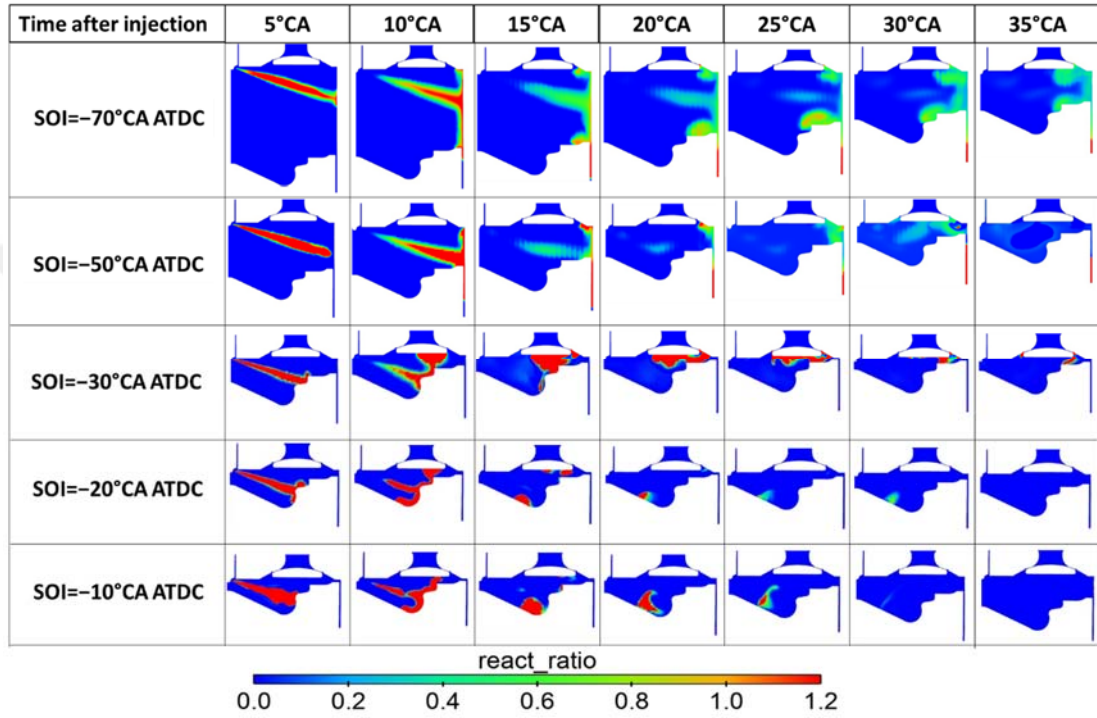


Figure 4.17: RER distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of $\text{SOI}=70^\circ\text{CA}$, $\text{SOI}=50^\circ\text{CA}$, $\text{SOI}=30^\circ\text{CA}$, $\text{SOI}=20^\circ\text{CA}$ and $\text{SOI}=10^\circ\text{CA}$ BTDC.

Figure 4.18 shows temperature distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of $\text{SOI}=70^\circ\text{CA}$, $\text{SOI}=50^\circ\text{CA}$, $\text{SOI}=30^\circ\text{CA}$, $\text{SOI}=20^\circ\text{CA}$ and $\text{SOI}=10^\circ\text{CA}$. In early injection events of $\text{SOI}=70^\circ\text{CA}$ and $\text{SOI}=50^\circ\text{CA}$ BTDC, auto-ignition starts on the richer zones closed to stoichiometry due to fuel wall impingement. These are the regions of below the valves, and inside the crevice volume. The temperature of the auto-ignition ranges between 1250-1750K, which is temperature of the combustion is quite lower than high temperature combustion of retarded injection events. In the squish region, splashed droplets that are splashed from the walls, generates a fuel richer region as they evaporate. Therefore, higher combustion temperature occurs due to richer AFVM leading to an increase

between 2000-2500K. Conversely, in the retarded injection events of SOI=30°CA, SOI= 20°CA, and SOI=10°CA BTDC, combustion occurs as expected in conventional diesel combustion. At SOI=30°CA BTDC, most of the spray jet is directed above the piston edge, high temperature combustion occurs inside the squish region. In retarded injection events of SOI=20°CA and SOI=10°CA BTDC, the fuel splits into two stream and directs into piston crown and above the stepped lip region. Combustion is controlled by diffusion, and the flame temperature reaches up 3600K, depending on the AFVM and equivalence ratio.

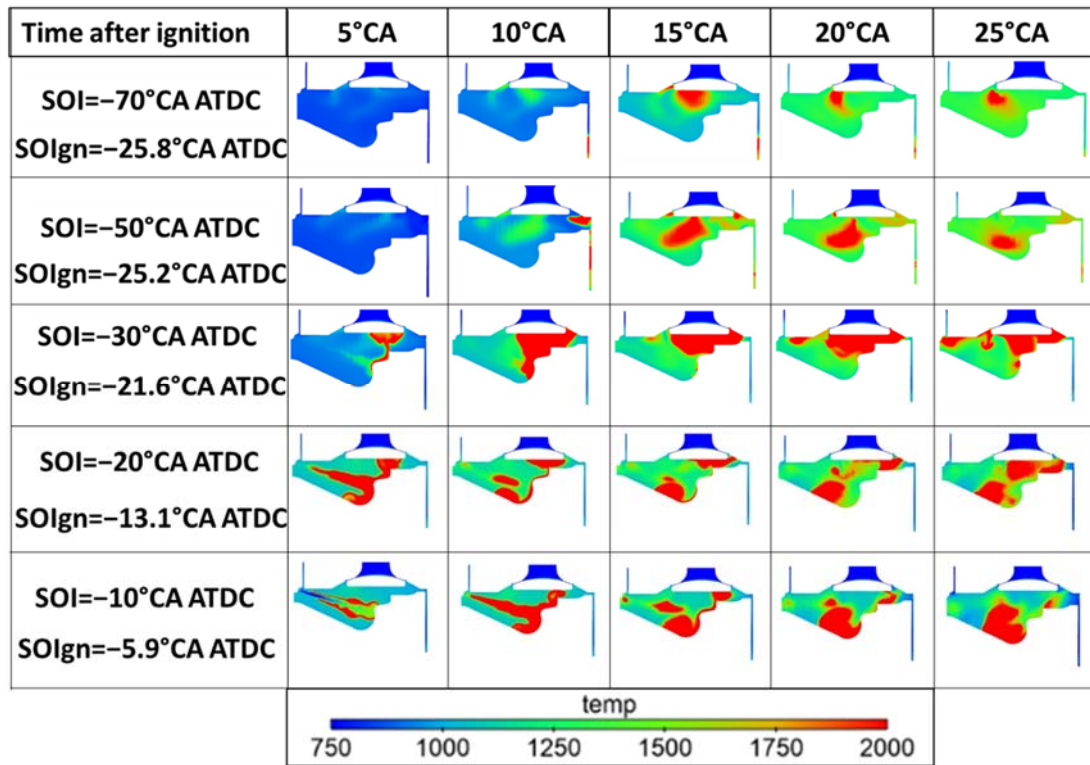


Figure 4.18: Temperature distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

Figure 4.19 shows NO_x distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC. In early injection events of SOI=70°CA and SOI=50°CA BTDC, extremely low NO_x production occurs because the mixture is too lean, and combustion takes places in low temperature. In the retarded injection events of SOI=30°CA, SOI=20°CA, and SOI=10°CA BTDC, more NO_x is produced due to richer AFVM in

the diffusion combustion zone. High temperature combustion triggers the production of the NO_x production on the oxygen rich surroundings of the flame.

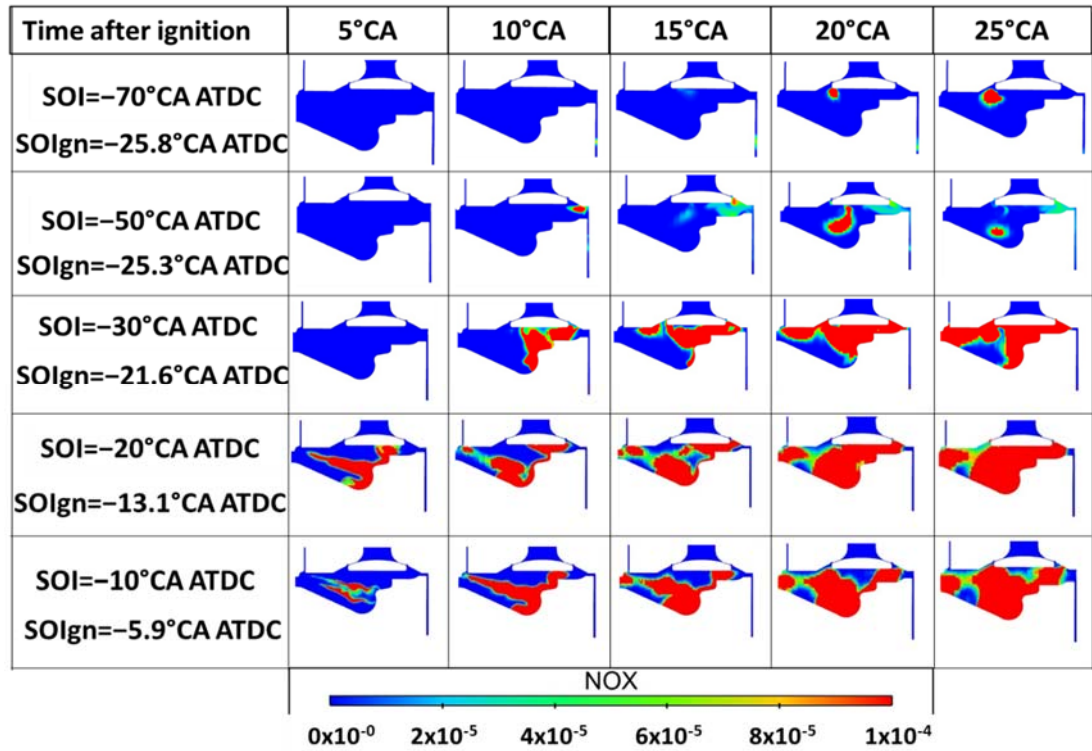


Figure 4.19: NO_x distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

Figure 4.20 shows soot distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC. In early injection events of SOI=70°CA and SOI=50°CA BTDC, soot production rate is gradually lower compared to high temperature combustion cases due to very lean combustion events. Additionally, soot particles are separated due to uniformity of AFVM. In the retarded injection events of SOI=30°CA, SOI=20°CA, and SOI=10°CA BTDC, soot formation is more concentrated inside the spray vapor core and production rate is extremely high due to the over-rich condition inside this region. On the other hand, high temperature and the oxygen availability surrounding the flame propagation zone results a high oxidation rate of soot particles. Overall, exhaust soot emissions are considerably low in retarded injection cases compared to advanced injection strategy.

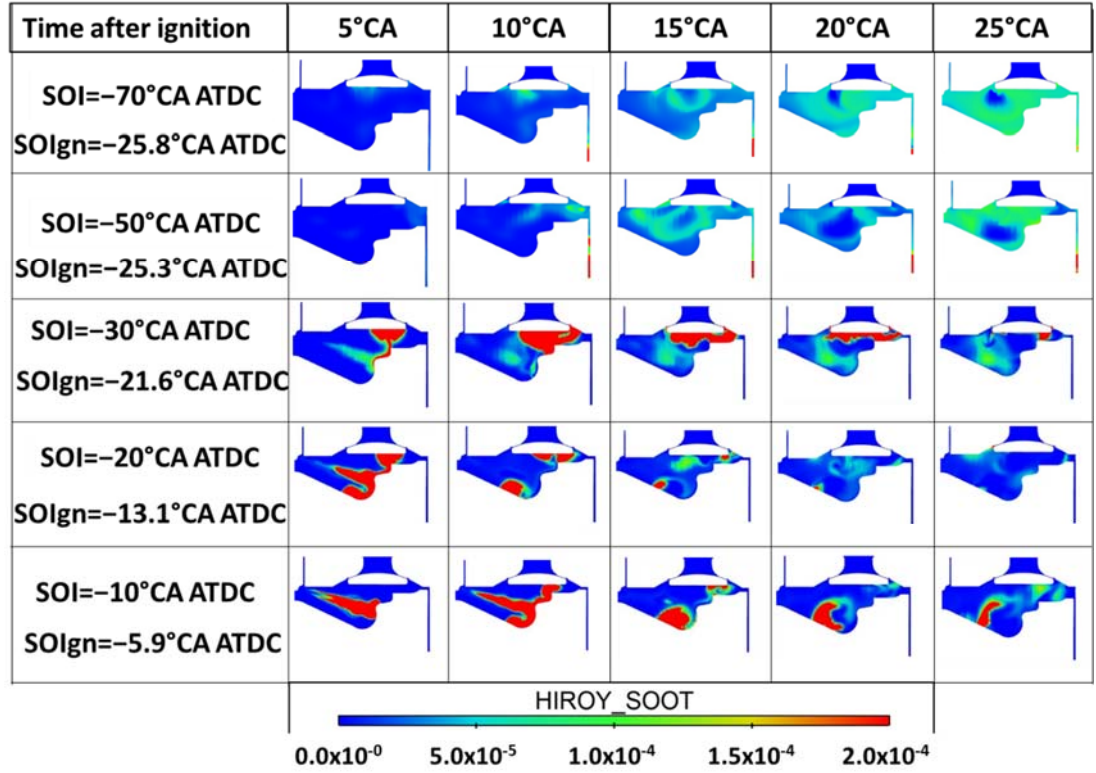


Figure 4.20: Soot distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

Figure 4.21 shows soot distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

CO emissions is extremely low in conventional diesel operation. On the other hand, significant amount of CO can be produced due to low temperature and in-complete combustion in very advanced injection strategies. CO is an intermedia species that, can be produced above 1000K temperature and it is chemically decomposed to CO₂ within the oxygen availability and high temperature conditions above ~1800K.

Therefore, CO transformation to CO₂ is not very sufficient in early injection events of SOI=70°CA and SOI=50°CA BTDC, due to low temperature combustion activities. In the retarded injection events of SOI=30°CA, SOI=20°CA, and SOI=10°CA BTDC, the rich AFVM in the downstream of spray undergoes premixed phase combustion, resulting in the formation of CO. However, this CO is subsequently oxidized to CO₂ under oxygen availability and high temperature combustion of between 1800-3500K.

Therefore, extremely low CO seen in the exhaust means that combustion is fully completed.

Emission, performance, and combustion specific outputs of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC are summarized in **Table 4.4**.

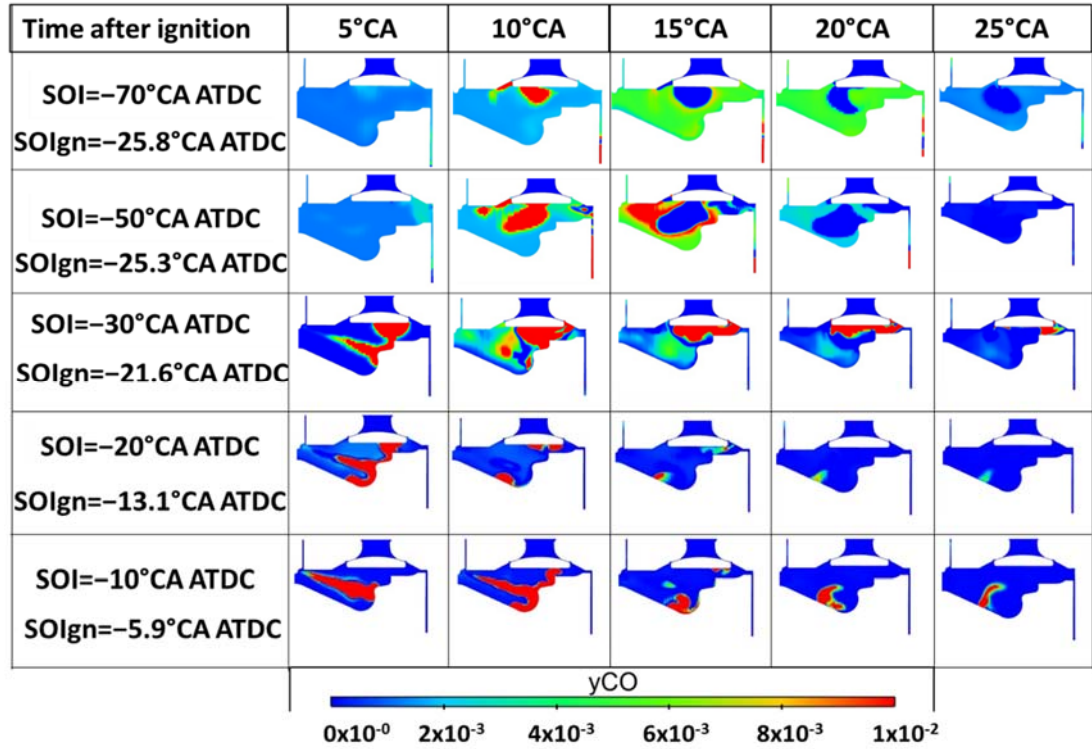


Figure 4.21: CO distribution on section plane through the spray center after 5, 10, 15, 20, 25, 30, 35°CA of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

Table 4.4: Summary of emission, performance, and combustion specific outputs of SOI=70°CA, SOI=50°CA, SOI=30°CA, SOI=20°CA and SOI=10°CA BTDC.

SOI [°CA BTDC]	70	50	30	20	10
Spray Penetration Length [mm]	>65	>65	44.8	42.6	29.8
Ignition Delay [°CA]	44.2	24.7	8.4	6.9	4.1
Start of Ignition [°CA]	25.8	25.3	21.6	13.1	5.9
Combustion Efficiency [%]	58.5	84.3	98.9	99.8	99.9
IMEP [bar]	1.99	2.34	3.23	3.64	3.89
NO _x [ppm]	4.04	54.8	3533.3	2368.6	1336.7
Soot [ppm]	147.8	206.8	20.5	13.6	17.1
CO [ppm]	134.3	935.0	22.4	12.6	16.4

4.5. Effect of Spray Inclusion Angle (SIA) on Engine Performance and Emissions

In early injection strategies, the ambient pressure and temperature are not sufficient as the piston is not complete the compression to execute an efficient break-up and evaporation mechanism, that easily penetrates the combustion chamber. Poor break-up and atomization cause a coarser droplet size and spray core is not expanded in the conical direction due to lower drag force generated by low combustion chamber density. Inadequate evaporation rates due to lower temperature resulting ineffective AFVM formation. Furthermore, in very advanced injection cases, there could a be direct spray wall interaction occurred in the liner, piston or crevice region depends on SOI and SIA. Based on CFD simulations, $SIA=146^\circ$ and injection pressure of 800 bar, if the SOI is advanced 30°CA BTDC , it can cause some of the fuel to not evaporate properly and instead stick to the cylinder wall. This can cause problems with a specific type of combustion called PCCI.

Alternatively, by reducing the SIA, it is feasible to resolve the issue of wall impingement of Early Single-Injection (ESI). This approach facilitates the formation of AFVM without any fuel impingement on cylinder liner over extended spray tip penetration lengths. As a result, advanced injection strategy increases the spray tip penetration length, using a narrow SIA can reduce or fully eliminate the spray wall impingement [145].

In this study, CFD simulations are used to examine the impacts of SIA on various parameters such as STPL, spray wall impingement, AFVM formation, and engine performance and emissions for ESI strategy. Specifically, the study analyzed the effects of spray wall interaction of very advanced injection strategies in a CI engine, utilizing various SIAs ranging from 80° to 146° . The injection timing of -50°CA ATDC was chosen due to its ability to reduce NO_x emissions and increase CE compared to late-injection cases. **Figure 4.22** illustrates fuel spray penetration route inside the combustion chamber for $SIA=146^\circ$, $SIA=140^\circ$, $SIA=130^\circ$, $SIA=120^\circ$, $SIA=100^\circ$ and $SIA=80^\circ$, under ESI with piston position at 50°CA BTDC , respectively.

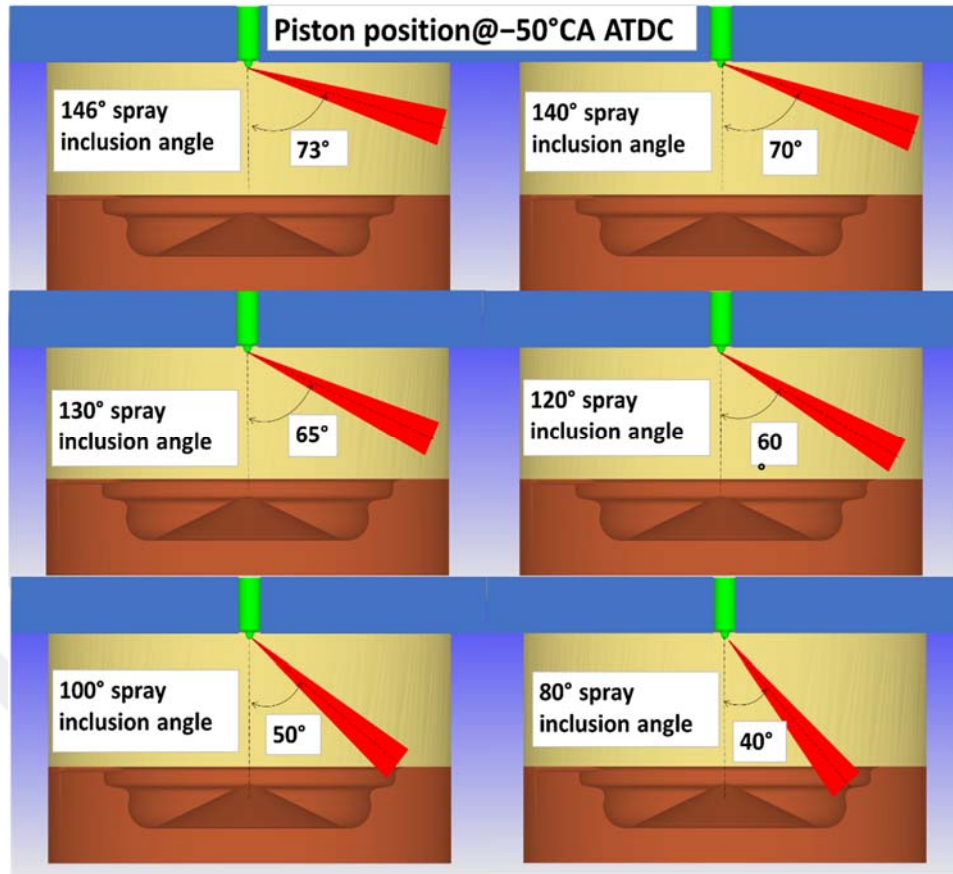


Figure 4.22: Fuel spray penetration route inside the combustion chamber for SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80°, under ESI with piston position at 50 °CA BTDC.

In **Figure 4.23**, the in-cylinder pressure histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80° at ESI of SOI=50°CA BTDC are displayed. According to the results, peak firing pressure is obtained with an SIA of 100°, followed by those with SIAs of 80° and 120°. Conversely, the lowest peak firing pressures are obtained above SIA=120°.

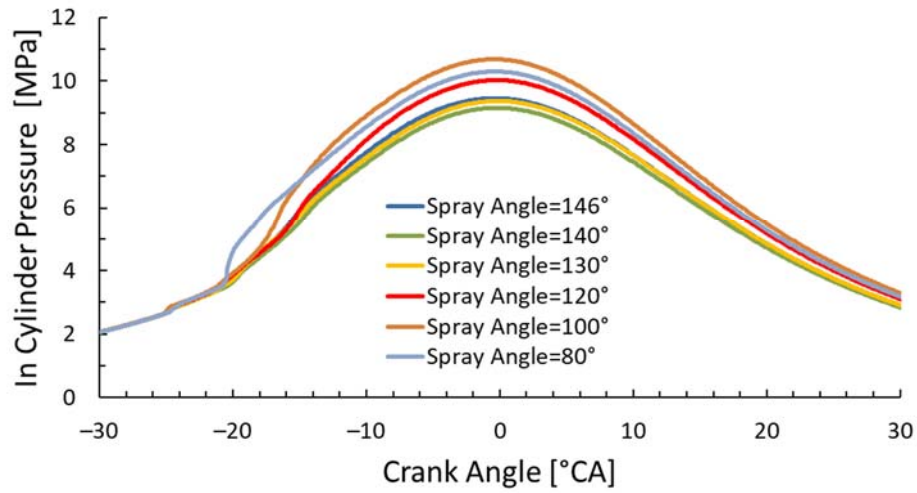


Figure 4.23: In-cylinder pressure histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80°, for SOI=50°CA BTDC.

In **Figure 4.24**, Apparent HRR histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80° at ESI of SOI=50°CA BTDC are shown. Interestingly, ID remains unaffected by SIA since auto-ignition occurs around -26 °CA ATDC regardless of the SIA value. However, the apparent HRR history varies significantly depending on the SIA used. Specifically, highest peak apparent HRR at -20 °CA ATDC in SIA=80°, and second peak in the apparent HRR is observed at -16.5 °CA ATDC in SIA=100°.

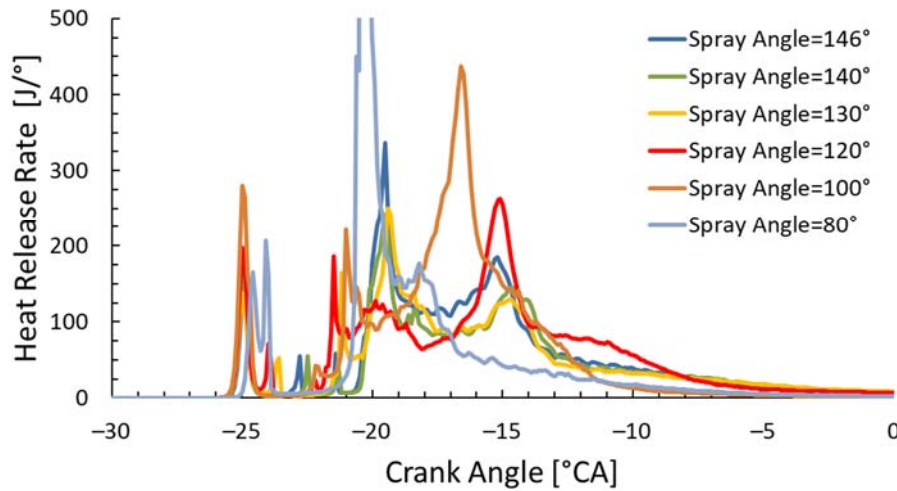


Figure 4.24: Apparent HRR histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80°, for SOI=50°CA BTDC.

Figure 4.25 shows the liquid fuel mass of the spray histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80°, for SOI=50°CA BTDC. By using narrow SIA, a homogeneity of the fuel can be utilized to target the fuel spray targeted on the edge of the piston to split the fuel into two streams. The results show that, liquid mass content of the spray is found to be the lowest for a 100° SIA, followed by an 80° SIA.

Moreover, analysis of the in-cylinder air motion in a planar section through the cylinder axis reveals the presence of clockwise and counter-clockwise vortices in the piston bowl and squish region, respectively. These vortices facilitate an air motion to increase the uniformity of spray droplets in the upper and lower fuel streams, leading to a significant improvement in the AFVM formation process. The two highest apparent HRR peaks are observed for SIA=100° and SIA=80°, as these sprays contain the least liquid content. In contrast, the lowest apparent HRR is seen of SIA=130°, spray impingement on cylinder walls.

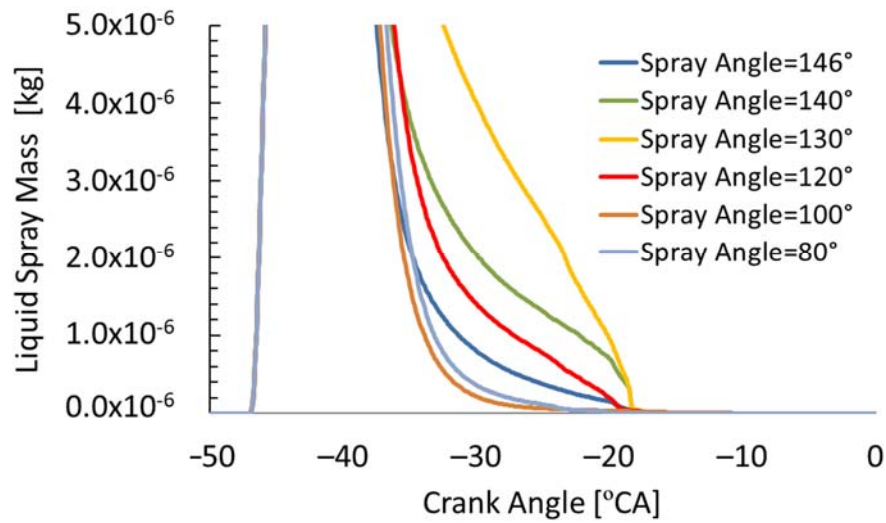


Figure 4.25: Liquid fuel mass of the spray histories of SIA=146°, SIA=140°, SIA=130°, SIA=120°, SIA=100° and SIA=80°, for SOI=50°CA BTDC.

Figure 4.26 illustrates STPL histories of spray penetration from the spray center of various SIA for SOI=50°CA BTDC. STPL experiences a reduction as SIA decreases. Cylinder liners are impinged by sprays with an SIA of 120° or greater, while piston crown and stepped lips are interacting with sprays in SIA of 80° and 100°, respectively.

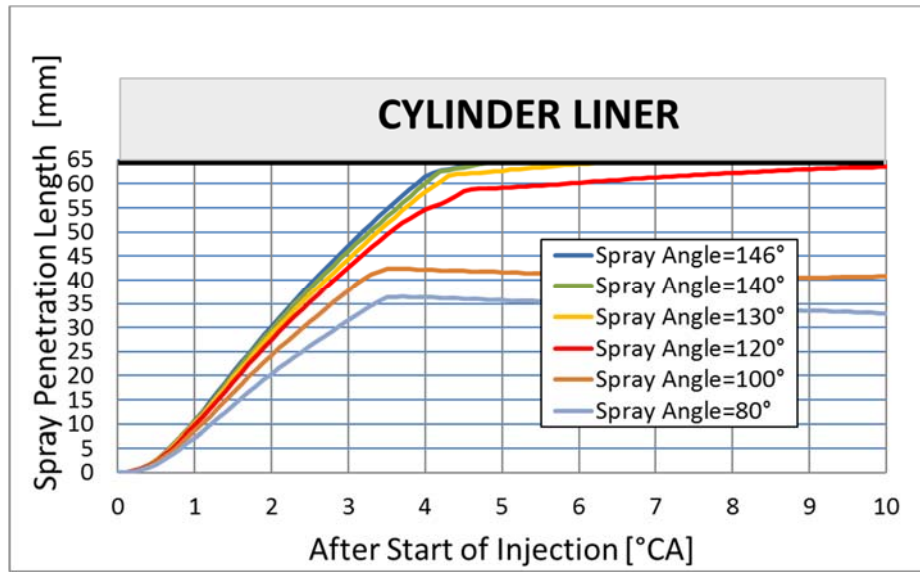


Figure 4.26: STPL histories of spray penetration from the spray center of various SIA for SOI=50°CA BTDC.

To demonstrate the impact of various spray angles, distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI. **Figure 4.27**, **Figure 4.28**, **Figure 4.29**, **Figure 4.30**, **Figure 4.31** shows spray penetration and RER for SIAs of 140°, 130°, 120°, 100°, and 80°. Specifically, when the SIA is 140°, there is interaction between fuel sprays and cylinder walls. Fuel accumulates on the liner and result an over fueled AFVM in the vicinity, which subsequently transforms into a lean mixture before auto-ignition. However, the combustion of this rich FVAM within the crevice at a low temperature and poor oxygen concentration triggers CO production.

Fuel sprays directly hits on the flat piston surface, accumulates in a liquid fuel form. Fuel droplets then spreads through piston surface and directs into the combustion chamber walls, with some of it moving towards the cylinder head and the rest entering the crevice in the case of SIA=130°. As the combustion chamber temperature increases, the liquid films evaporate, resulting in the formation of over fueled regions between piston surface and cylinder head and some of the fuel accumulates in the crevice volume. Additionally, a lean mixture is produced near the soot-in-oil rim

region, as most of the droplets partially evaporate until impinging on the soot-in-oil region and fail to auto-ignite.

In $SIA=120^\circ$, fuel sprays impinge the piston edge and divided into two branches. Lower stream moves towards the piston bowl and increase the uniformity of AFVM with the help of the vorticity inside the piston, while the other moves towards the cylinder liner. The upper part of the stream splits and partially moves up the liner towards the cylinder head, some of the fuel moves into the crevice volume.

In $SIA=100^\circ$, the fuel spray penetrates the stepped lip region of the piston and splits into two branches as seen in $SIA=120^\circ$. Upper stream turns its direction by the geometry of the stepped lip into the under-valve region, while the lower stream directs into the piston crown. The fuel vapor follows the geometry of the piston bowl shape and increases the AFVM uniformity. Spray penetration on the stepped lip region helps AFVM preparation before it ignites, which reduces the amount of carbon monoxide emissions [145].

Furthermore, a narrow SIA leads to a shorter STPL, resulting in lower levels of soot emissions because of increased formation of AFVM. When the $SIA= 80^\circ$, the fuel spray impinges inside the piston crown and splashes. With the help of the vortex inside the piston crown generated by the bowl geometry interaction with the air, creating an accumulated large and rich AFVM region. As a result, the narrow SIA prevents the spray from hitting the cylinder liner, making it an effective approach for the ESI strategy [146].

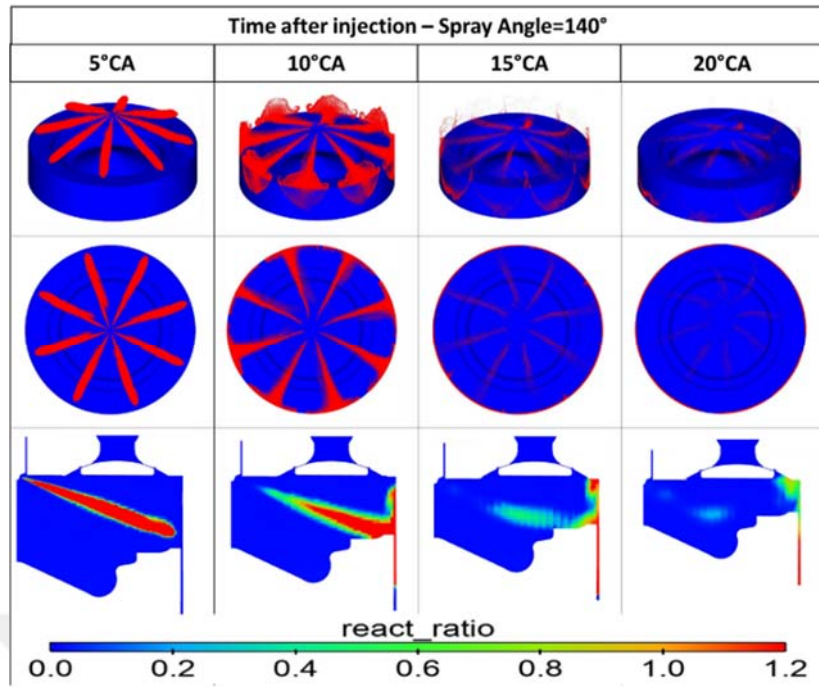


Figure 4.27: Distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI of SIA=140°.

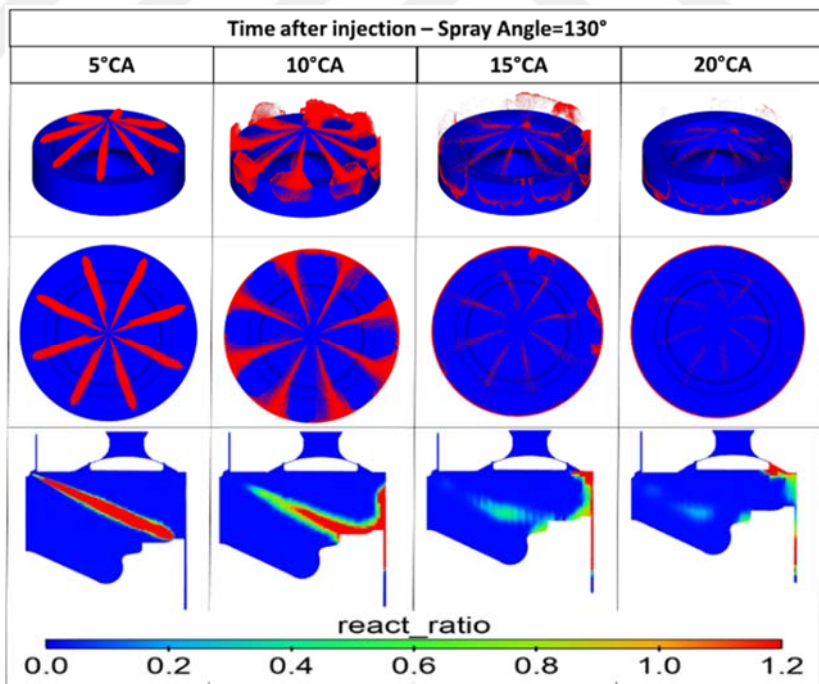


Figure 4.28: Distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI of SIA=130°.

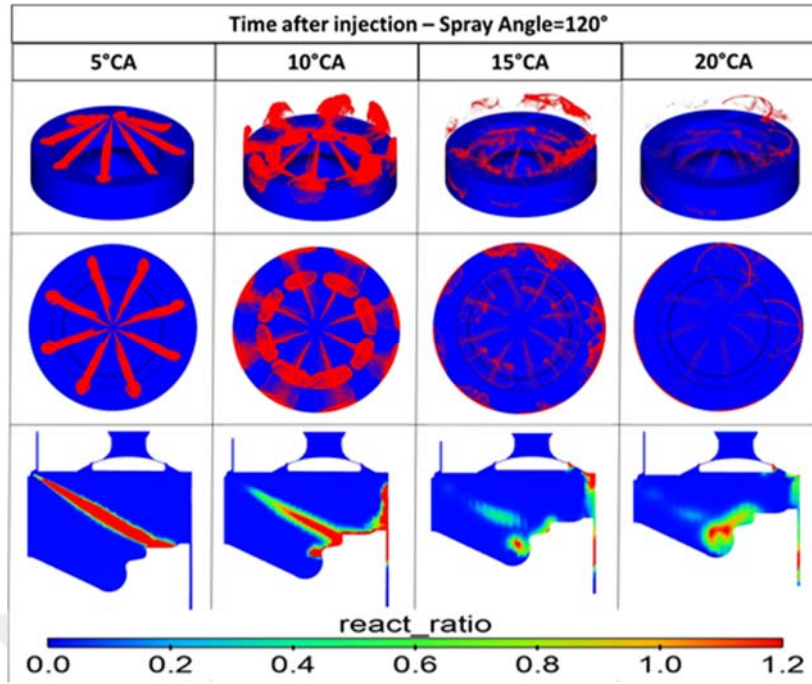


Figure 4.29: Distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI of SIA=120°.

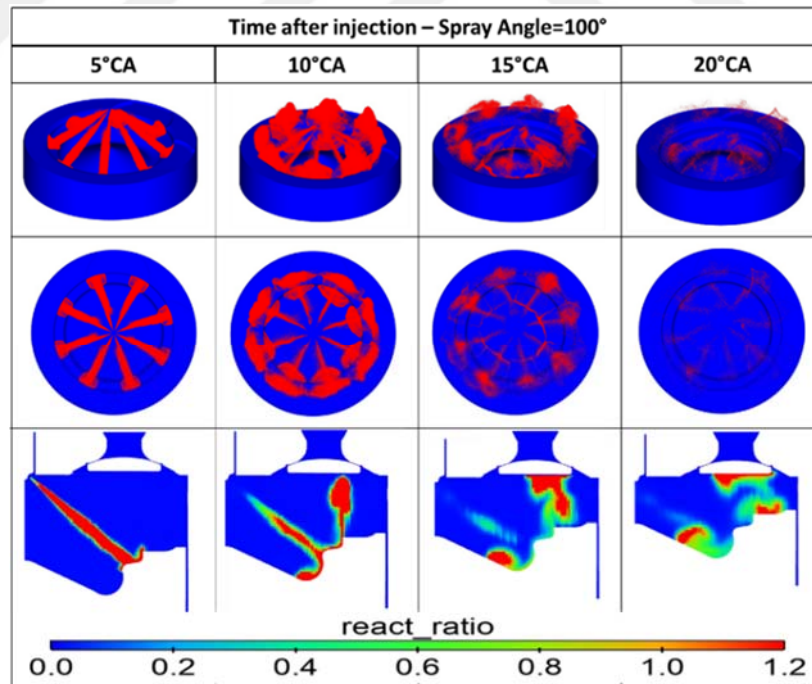


Figure 4.30: Distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI of SIA=100°.

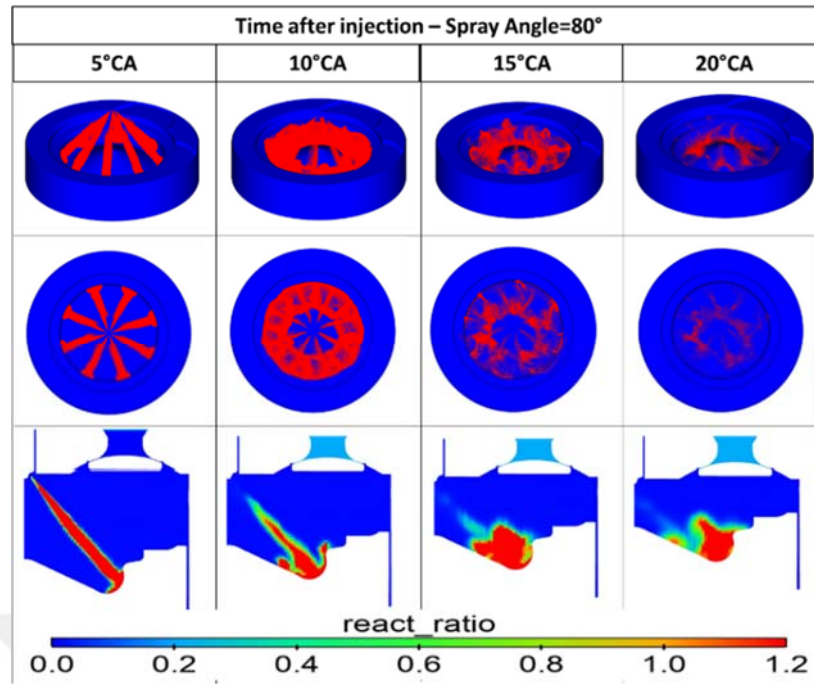


Figure 4.31: Distribution of spray droplets in isometric and top views, and distribution of reaction equivalence ratio contour in a section plane through the spray center after at various °CA after SOI of SIA=80°.

Figure 4.32, Figure 4.33, Figure 4.34, Figure 4.35, Figure 4.36 show contour plots distribution of temperature, NO_x , and soot, of SIA=140°, SIA=130°, SIA=120°, SIA=100°, and SIA=80°. These plots are presented on section plane through the spray center after of 5°CA, 10°CA, 15°CA, and 20°CA after SOIgn.

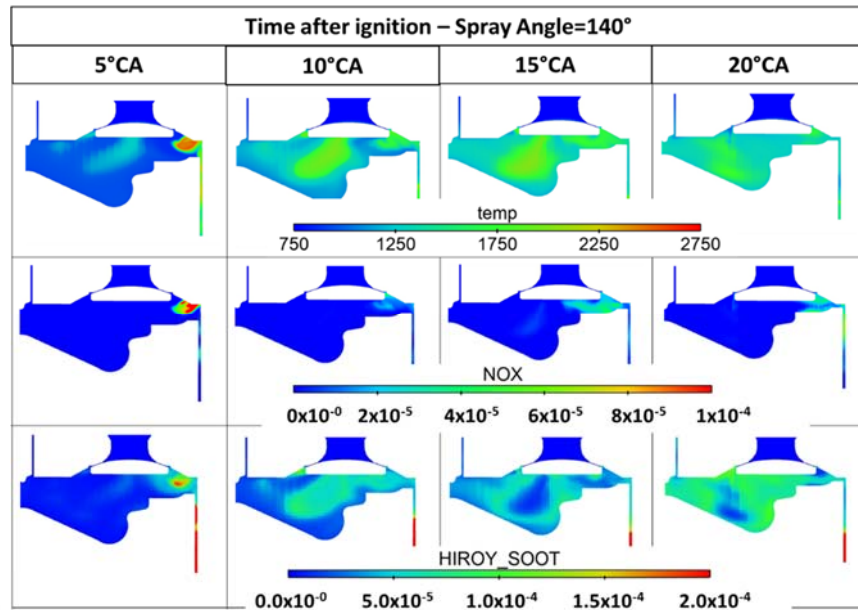


Figure 4.32: Temperature, NO_x, and soot distribution on section plane through the spray center after at various °CA after SOI of SIA=140°.

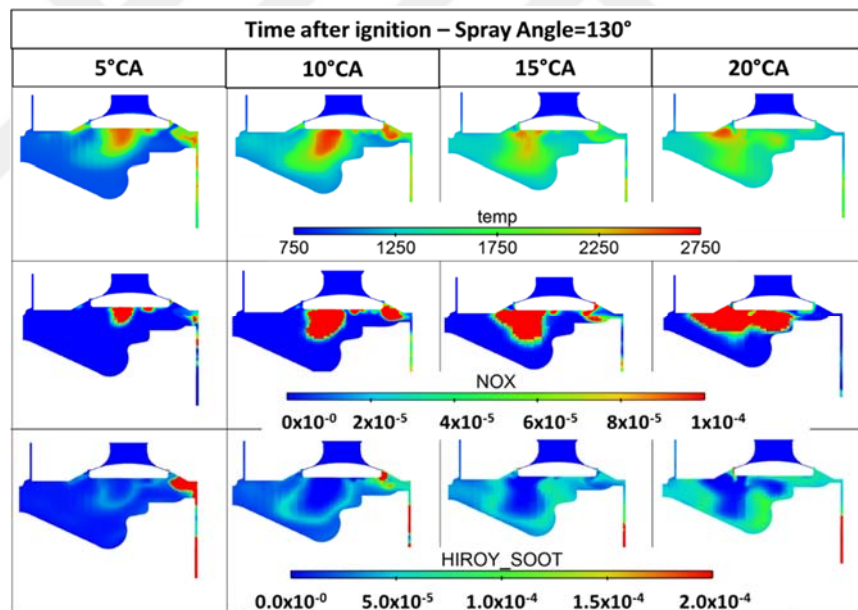


Figure 4.33: Temperature, NO_x, and soot distribution on section plane through the spray center after at various °CA after SOI of SIA=130°.

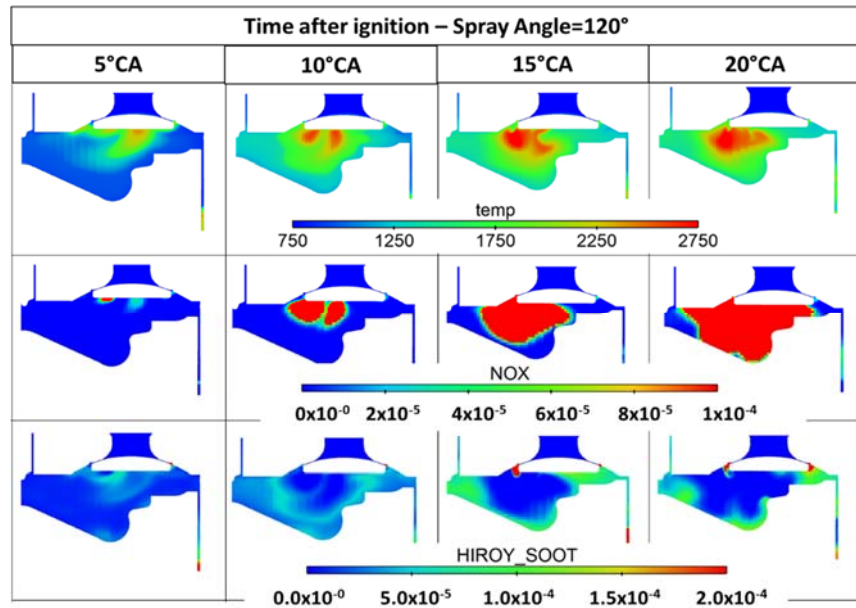


Figure 4.34: Temperature, NO_x, and soot distribution on section plane through the spray center after at various °CA after SOI of SIA=120°.

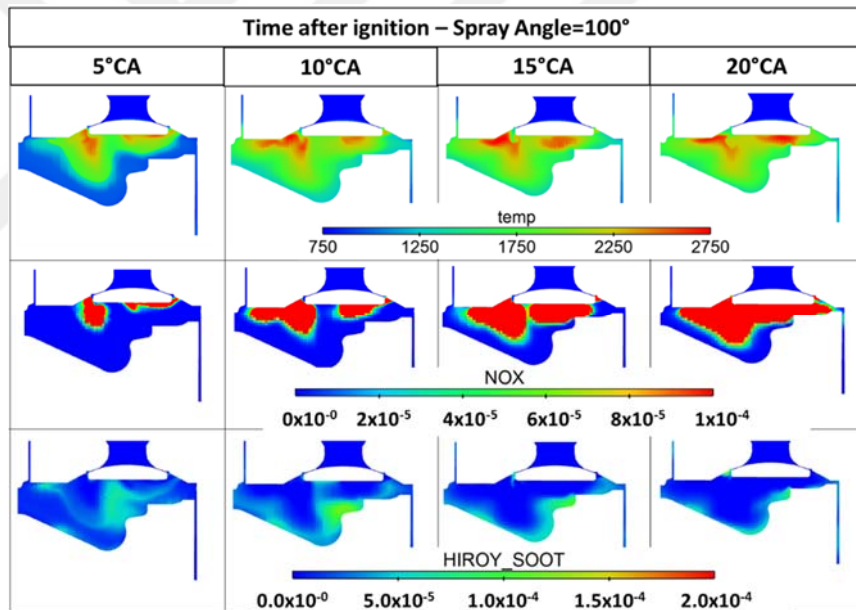


Figure 4.35: Temperature, NO_x, and soot distribution on section plane through the spray center after at various °CA after SOI of SIA=100°.

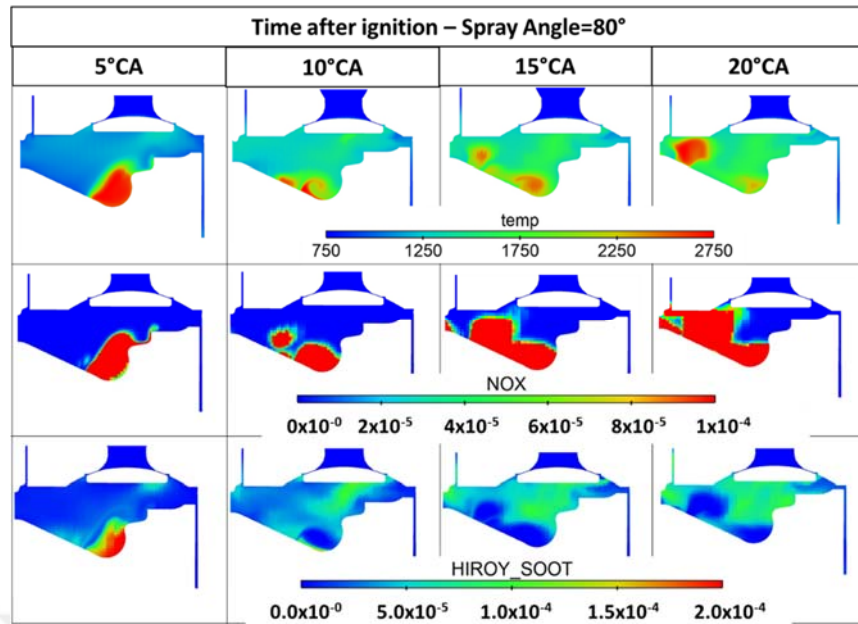


Figure 4.36: Temperature, NO_x, and soot distribution on section plane through the spray center after at various °CA after SOI of SIA=80°.

The results of this study show that an SIA=140° leads to minimal NO_x formation in combustion chamber and the auto-ignition zone in the squish volume. This is due to excessive accumulation of fuel into the liner and the squish region and poor mixing of AFVM to generate a lean zone of premixed combustion, which only occurs in the squish region, where combustion temperature values are between 1750-2250 K. As a result, SIA=140° produces the lowest NO_x emissions compared to the other SIA cases investigated.

However, impingement of sprays in cylinder liners can result in the formation of soot excessively. Over fueled of the regions that are generated by the splashed and rebounded droplets inside the combustion chamber causes excessive soot production after auto-ignition of these high temperature rich zones about 2250K. In addition, the oxidation rate of the soot is low compared to production rate due to low temperature about 1350K on the oxygen rich outside that soot is transported to this zone.

In SIA=130°, combustion occurs in two stages. Firstly, the lean AFVM located under valve region ignites spontaneously, and then flame propagates into the piston bowl and towards the cylinder axis area by the vorticity of the mixture above the flame deck area. However, NO_x emissions increase due to rich AFVM zones of high temperature and a having a large volume of premixed flames. The locations where soot is formed

and consumed are similar to those observed in an SIA=140°. Some of the soot particles, produced in the fuel rich regions, is carried along with the air motion inside the engine and then oxidized by rapidly in the regions that flame temperatures of 1750 to 2750K. On the other hand, in the regions of the temperature level is below 1500K, soot particles are not oxidized even the oxygen concentration is sufficient.

Soot emissions are at their most extreme in SIA=130°. This is because a significant amount of soot is produced, while the amount of soot oxidation is minimal. This is because lean-premixed flames tend to linger in the upper portion of the combustion chamber.

In SIA=120°, the fuel sprays impinge on the piston edge and splits into two branches. The upper jet moves onto the flat surface of piston, reaches the squish region, and then turn towards to the region below flame deck by the effect of the vortex in the squish region generated by the piston motion in the compression stroke.

The lower stream enters the piston crown and flows the crown geometry. In this region, a uniform AFVM is developed by the help of the vortex in the clockwise direction generated by the piston bowl geometry in the compression stroke.

Both branches mix with the air and become leaner as they spread tangentially.

As the temperature in the combustion chamber rises, too lean AFVM starts to ignite in the region below the valves, and flame propagates towards the fuel rich zones of piston bowl. Temperature levels are ranging between 1750-3000K in the combustion zone which is higher than SIA=140°.

On the other hand, with a 120° SIA, combustion of minor, fuel-rich mixture around the valve edges and in the crevice due to evaporation of splashed fuel droplets and drained fuel films from the cylinder liner contribute to increased soot production during combustion.

On the other hand, for SIA=120°, soot is formed by the surroundings of the fuel propagation of rich AFVM regions. These particles are transported to the center of cylinder and the particles in the squish region increase the soot production due to low local temperature levels around 1200-1500K. In addition, splashed droplets near valve edges and accumulated fuel in the crevice region causes soot formation.

However, soot emissions are reduced by almost 50% compared to a 140° spray angle due to decreased soot formation in the crevice and increased soot oxidation in the much larger lean-premixed combustion zone within the piston bowl. On the other hand, $\text{SIA}=120^\circ$ can produce nearly half of the soot emissions compared to $\text{SIA}=140^\circ$. This is because, very low fuel accumulates in the crevice volume and better homogeneity of AFVM in the lean-combustion zone.

In $\text{SIA}=100^\circ$, ignition starts from the edges of the valve region and flame propagates rapidly into both radial direction and into the piston crown because of the uniform AFVM generation on the large volume. The success of the AFVM homogeneity is due to the fuel jet impingement of the stepped lip of the piston. Fuel spray is split into the two branches and meet with unburnt air in the piston crown and squish region. The temperature level of $\text{SIA}=100^\circ$ in the flame core is between 2000-3000 K, and NO_x emissions are slightly lower due to better homogeneity and leaner combustion temperature compared to $\text{SIA}=120^\circ$.

In $\text{SIA}=100^\circ$, soot is produced in areas that are fuel-rich, such as under the exhaust valves and inside the piston crown, with a ratio of approximately 2.0. However, when the mixture is more homogeneous due to the absence of these rich areas, soot formation decreases, while the temperature range of the premixed combustion flame increases between 1750-3000 K. Compared to larger spark ignition angles, the amount of soot emitted from the engine is significantly reduced since higher temperatures and larger premixed flames lead to more efficient soot oxidation. This is shown in **Figure 4.35**.

In the case of an SIA of 80° , the piston bowl experiences a notable increase in the volume of a rich AFVM zone, as the spray hits the curved portion of the bowl. However, tumble motion in the piston bowl prevents splashed droplets from reaching the top, resulting in an extremely lean mixture outside the bowl. This causes the rich FVAM to auto-ignite near the curved portion, followed by the propagation of a over fueled premixed flame along the inclined straight section towards the combustion chamber axis. Rich-premixed flame zone is much larger in size, with a combustion temperature level between 1750-3000 K, resulting to a gradually increase in NO_x emissions compared to lean-premixed combustion in larger SIAs. However, the initial formation of soot in the piston crown during rich combustion is efficiently eliminated by the uniform AFVM of high-temperature flame propagation as it travels towards the

cylinder centerline. This provides the lowest soot emissions compared to all the other SIA configuration analyzed.

NO_x and soot emission values of $\text{SIA}=140^\circ$, $\text{SIA}=130^\circ$, $\text{SIA}=120^\circ$, $\text{SIA}=100^\circ$, $\text{SIA}=80^\circ$ is shown in **Figure 4.37**. In wide angle SIAs, there is a significant amount of soot emissions despite achieving very low engine-out NO_x emissions. This is due to combustion occurring near the cylinder liner, resulting in quenched flames and excessive soot production from rich mixtures combusting at lower temperatures. Narrower SIAs, on the other hand, offer more uniform FVAM by targeting the piston bowl's stepped lip with spray, can provide a lean premixed high temperature combustion which leads superior reduction of soot emissions but a rapid rise in NO_x emissions. SIA of 80 and 100° achieves the extremely low exhaust soot emissions due to high temperature flame propagation and motion inside the combustion bowl which provides the conditions that required for soot oxidation. But it also leads to excessive NO_x emissions.

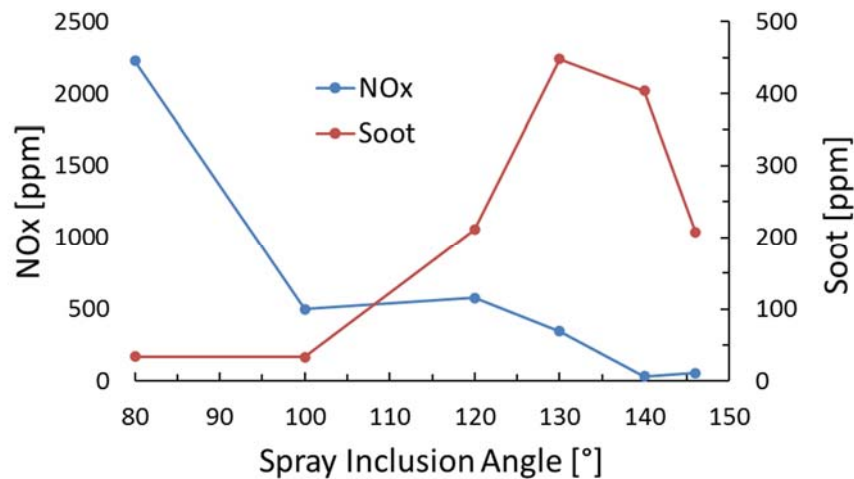


Figure 4.37: NO_x and soot emission values of $\text{SIA}=140^\circ$, $\text{SIA}=130^\circ$, $\text{SIA}=120^\circ$, $\text{SIA}=100^\circ$, $\text{SIA}=80^\circ$.

The engine-out CO emissions of engines, according to SIA, is shown in **Figure 4.38**. For wider SIAs, incomplete combustion in proximity to wetted cylinder walls leads to elevated levels of CO emissions [147]. In the case of ESI, a reduction in SIA targeting the stepped lip of the piston bowl leads to homogeneity of lean AFVM and better distribution of fuel in the combustion chamber to provide a high temperature combustion resulting a complete combustion and as a results ultra-low CO production.

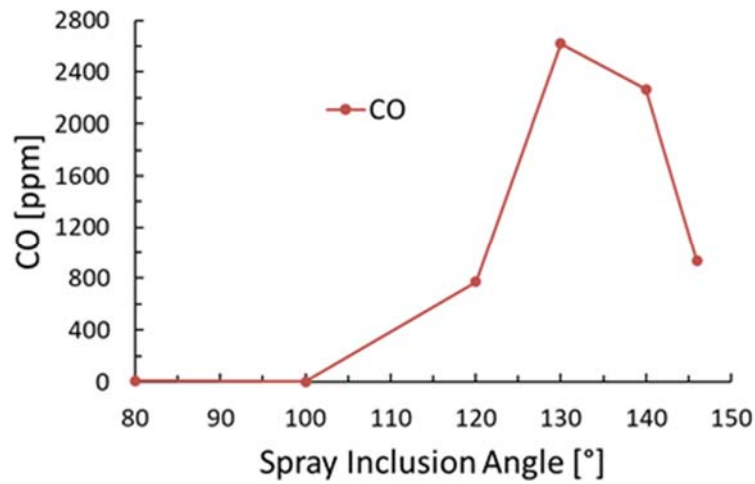


Figure 4.38: CO emission characteristics of various SIAs.

The CE and IMEP for different types of spark ignition engines are shown in **Figure 4.39**. Engines with wider SIA (146°, 140°, and 130°) have lower CEs (84.3%, 78.9%, and 81.5% respectively) compared to engines with narrower angles (120°, 100°, and 80°), which have higher CEs (91.3%, 97.8%, and 96.3% respectively). This is because incomplete combustion occurs in the wider SIA, due to poor mixing of fuel and air at low temperatures. The lowest CE is found in the engine with a 140° angle, where incomplete combustion occurs in both the squish region and crevice. Combustion temperatures levels are between 1500-2000 K, after the fuel spray impinges on the cylinder liner.

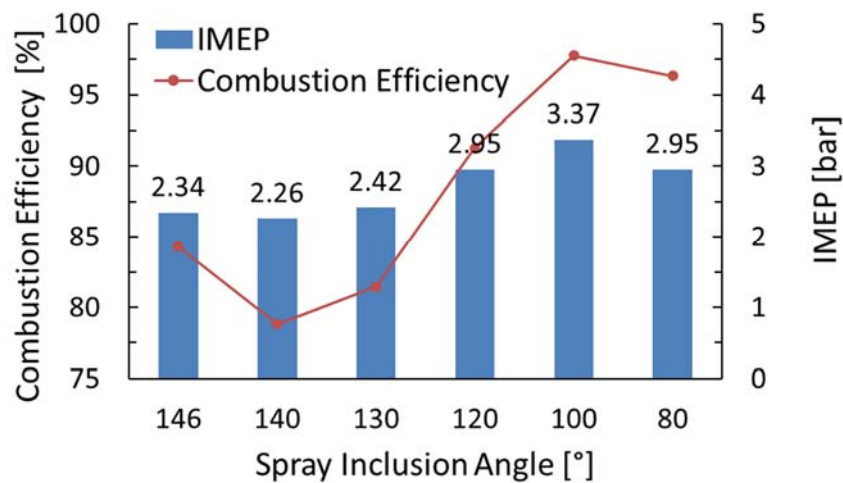


Figure 4.39: CE and IMEP for various SIAs.

The best combustion efficiency of 97.8% and peak firing pressure of 107 bar are achieved with SIA=100°. This is because of the use of high-temperature lean-premixed combustion of better homogeneity of AFVM. Combustion temperatures between 2250-3000 K where complete combustion occurs and eliminates UHC and soot production in the piston crown and squish region. To achieve this, the fuel spray is targeted at the tip of piston edge, creating a better homogeneity of AFVM in the combustion chamber and preventing spray impingement and eliminating any possibility of fuel to penetrate the crevice volume.

Results show that, SIA=100° achieves best IMEP and CE outputs. This is attributed to the spray being directed towards the edge of the piston crown, which avoids any impingement on the cylinder liner, resulting in optimal AFVM. On the hand, SIA=140° setting results in the lowest IMEP output of the spray impingement with the cylinder liner, resulting in excessive soot emissions and in-complete combustion due to insufficient air-fuel homogenization. STPL, CE, IMEP, NO_x, and CO values of various SIA's is shown in **Table 4.5**.

Table 4.5: STPL, CE, IMEP, NO_x, and CO values of various SIA's

Spray Inclusion Angle [°]	146	140	130	120	100	80
Spray Penetration Length [mm]	>65	>65	>65	63.3	42.4	36.2
Combustion Efficiency [%]	84.3	78.8	81.5	91.3	97.8	96.3
IMEP [bar]	2.34	2.26	2.42	2.95	3.37	2.95
NO _x [ppm]	54	34	345	575	498	2227
Soot [ppm]	206	403	447	210	33	33
CO [ppm]	935.0	2266	2620	770	2	8

4.6. Split Injection Strategy

4.6.1. Spray Penetration Analysis of Split Injection Strategy

The use of a split injection strategy is a viable approach for eliminating the issue of fuel spray interaction with cylinder surfaces for advanced injection across various engine operating conditions. Furthermore, when coupled with EGR, the splitting the main injection event can enhance AFVM, leading a reduction soot emission [148]. It has been observed that under the advanced injection strategy, the implementation of

EGR - exceeding 50% - can lead to significant reduction in the spray penetration length[149].

Furthermore, the implementation of EGR with injection the fuel spray into the edge of the stepped lip of the piston under PCCI conditions has been shown to significant reduction in both soot and NO_x emissions [147].

In addition, use of multiple injection in advanced injection strategy, low temperature of the premixed combustion can increase the auto-ignition event of the subsequent fuel sprays and promotes AFVM and high temperature combustion [150].

The current section of the study focuses on analyzing the impact of split injection on reducing spray wall wetting in advanced injection strategies. For this purpose, split injection event of SOI=-60°CA ATDC and SOI=-40°CA ATDC, respectively, are used. One-third and two-thirds of the fuel spray are directly injected into the cylinder during the first and second injections, respectively, resulting in a total fuel mass of 39 mg per cycle. The injection velocity profiles for both the first and second injections are in triangular shape, as illustrated in **Figure 4.40**. Injector test bench measurements are used to generate injection profiles.

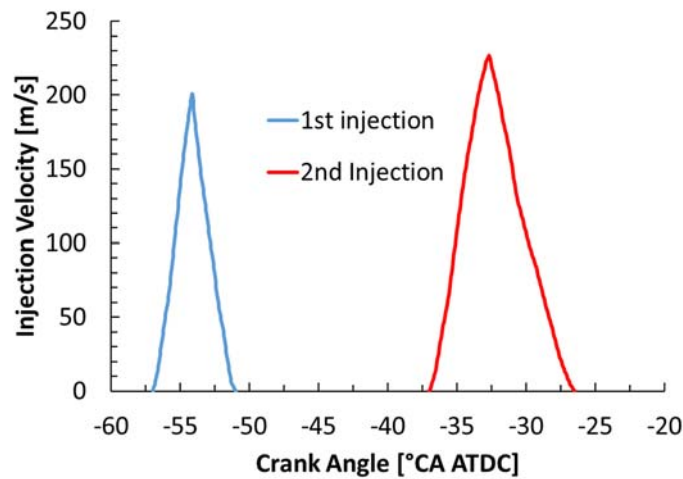


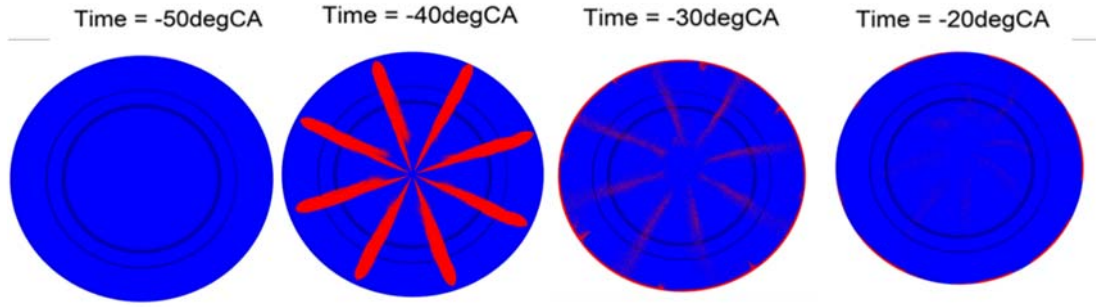
Figure 4.40: Velocity profiles of the first and second injection events.

In **Figure 4.41a**, it is observed the trajectory of the fuel sprays into the cylinder during a single main injection event at SOI=-50°CA. The liquid spray penetrates into the combustion chamber and impinges with the cylinder liner, with the high spray momentum preventing effective rotation in the swirl direction. **Figure 4.41b** presents

the reaction equivalence ratio contour-plot history in a plane intersecting the cylinder and spray axes. Most of the fuel vaporizes on the liner, inside the crevice area and under the cylinder head valves, as a result of the liquid spray impact in this region and fuel splashing under the valve region. Unfortunately, the fuel-air mixing is inadequate, resulting in an excessively rich region that can contribute to excessive HC build-up and soot emissions.

Figure 4.42a shows the history of the spray droplet penetration of the first and second fuel sprays into the cylinder on top view. After performing first injection, fuel sprays are deflected circumferentially by swirl motion inside the cylinder, therefore spray impingement on cylinder liner and accumulation in the crevice volume are reduced. In the second injection event, fuel sprays penetrate the region between neighboring of first injection sprays and impinge on the stepped lip of the piston bowl, splitting into two streams. The upper stream moves towards the region below flame deck and piston squish region, while the lower stream penetrates into the re-entrant region and follows the piston geometry in clockwise direction. **Figure 4.42b** shows the reaction equivalence ratio contour-plot history of the fuel vapor-air-gas mixture in a plane through the cylinder axis and a spray axis. The uniformity of the fuel vapor-air-gas mixture is significantly improved before the main combustion due to exposure to swirling fresh air and the dispersion of fuel droplets in both the squish volume and piston bowl.

a)



b)

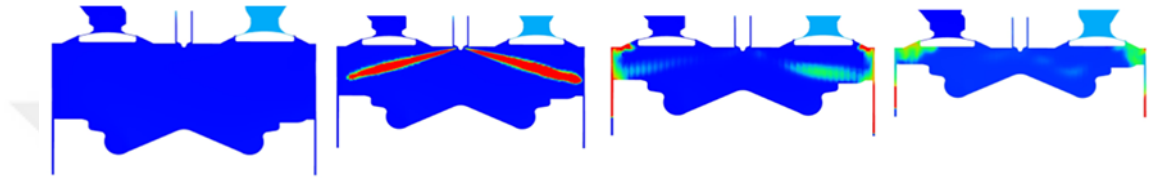
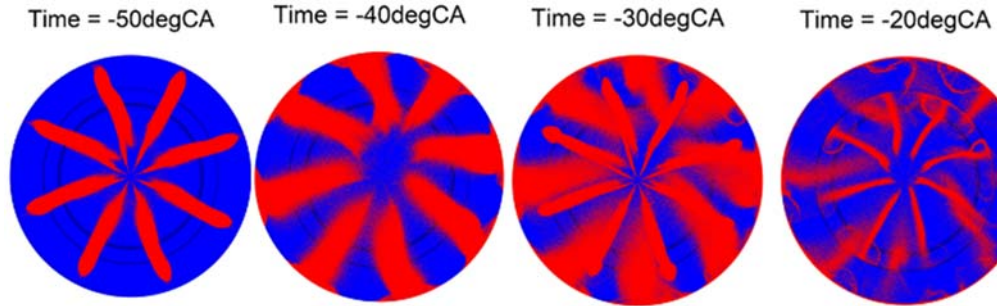


Figure 4.41: History of single injection event of $\text{SOI} = -50^\circ\text{CA}$ ATDC at piston positions of -50°CA , -40°CA , -30°CA , -20°CA ATDC a) Spray droplet distribution b) RER distribution.

a)



b)

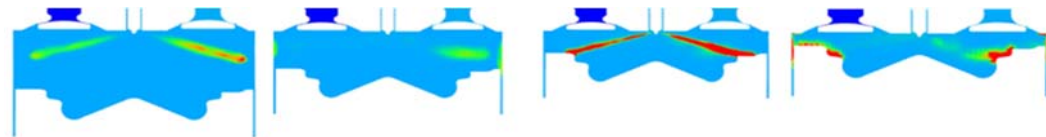


Figure 4.42: History of split injection event of $\text{SOI} = -60^\circ\text{CA}$ ATDC and $\text{SOI} = -40^\circ\text{CA}$ ATDC at piston positions of -50°CA , -40°CA , -30°CA , -20°CA ATDC a) Spray droplet distribution b) RER distribution.

As shown in **Figure 4.43**, history of STPL's is provided for single only and split injection strategies. Notably, both injection methods result with a spray wall

interaction. But using a split injection strategy is effective to reduce the amount of fuel impinging on the cylinder wall.

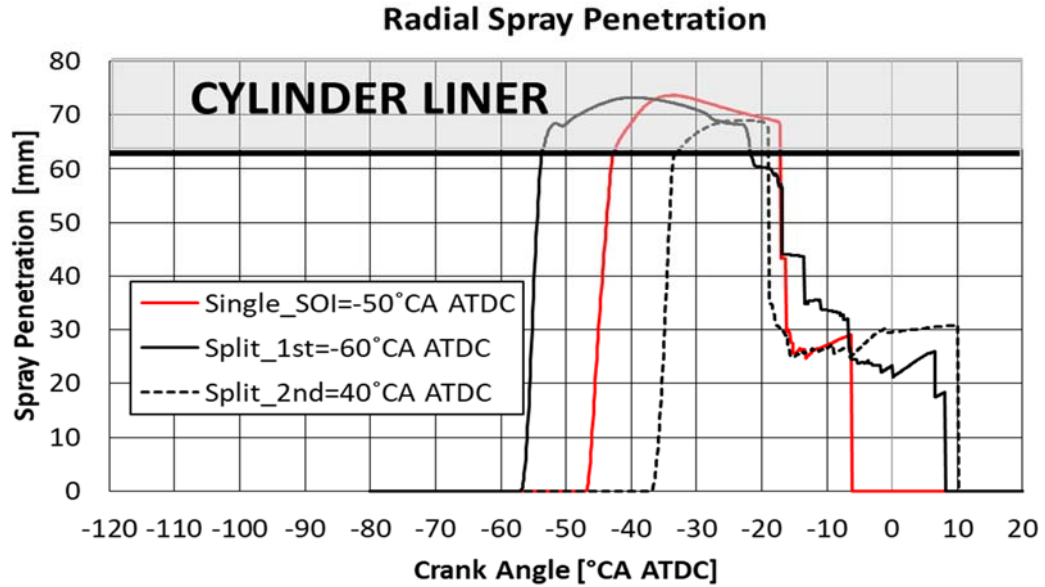


Figure 4.43: History of STPL's for single only and split injection strategies.

4.6.2. Split Injection Strategy with EGR

In this section, the impact of EGR is investigated in terms of combustion and performance characteristics of the split injection strategy. **Table 4.6** outlines the intake gas composition in various EGR rates. With increasing EGR rates, the oxygen mass concentration is dropped significantly, and CO₂ and H₂O concentrations are slightly increased. Composition of various EGR rates is used to provide initial conditions in the simulations. In addition, even in no-EGR conditions, the combustion chamber retains approximately 2.3% EGR gas due to residuals of the combustion volume of previous cycle. Residual gas concentration can be calculated by TDC volume and the geometric compression ratio.

Table 4.6: Intake air mass flow rate and gas concentrations for various EGR rates.

EGR Rate [%]	Intake Air Mass [kg/h]	Charged Gas Composition - [w%]			
		O ₂	N ₂	CO ₂	H ₂ O
0	92	0.210	0.769	0.002	0.001
30	64.4	0.209	0.765	0.018	0.007
50	46	0.182	0.759	0.042	0.017
70	27.6	0.119	0.745	0.097	0.040

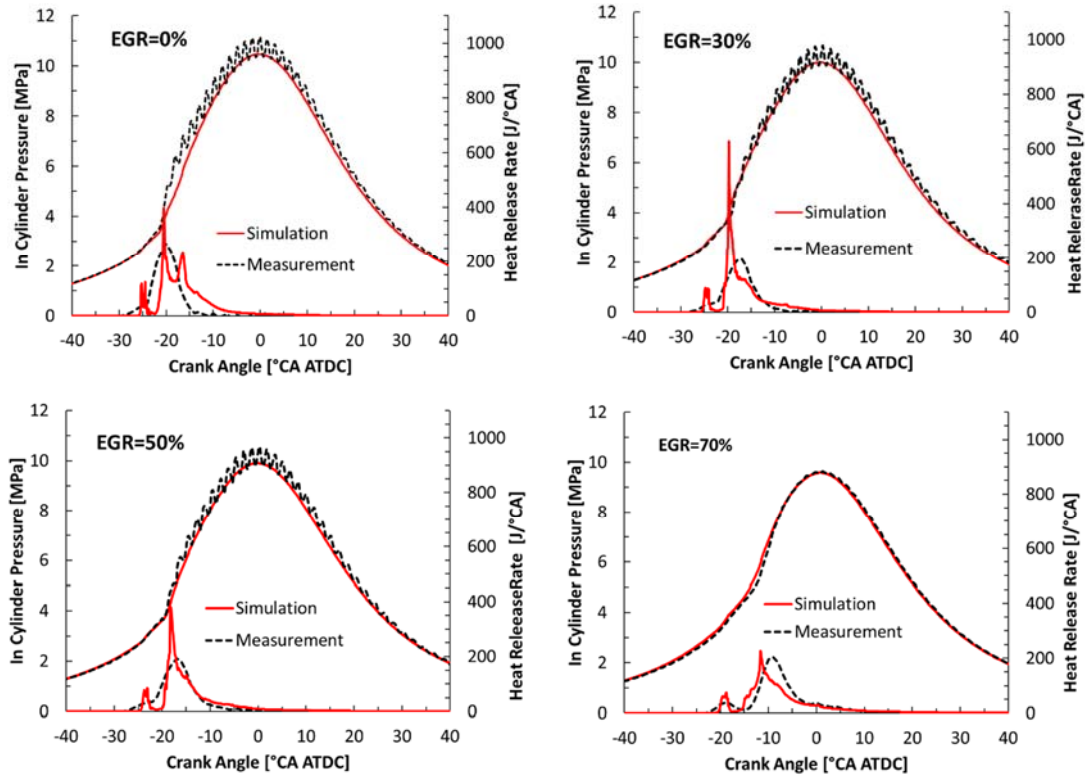


Figure 4.44: In-cylinder pressure and HRR histories for various EGR rates of split injection strategy.

As can be seen from **Figure 4.44**, the split injection strategy with various EGR rates was studied using both experimental measurements and 3D CFD simulations. The obtained in-cylinder pressure and AHRR histories were found to be in good agreement with the predictions of the CFD simulations. However, a slight discrepancy was observed in pressure histories between tests and the simulation during the combustion, which can be attributed to the fuel system pulsation causing a covariance of approximately 1% of the injected fuel mass per cycle.

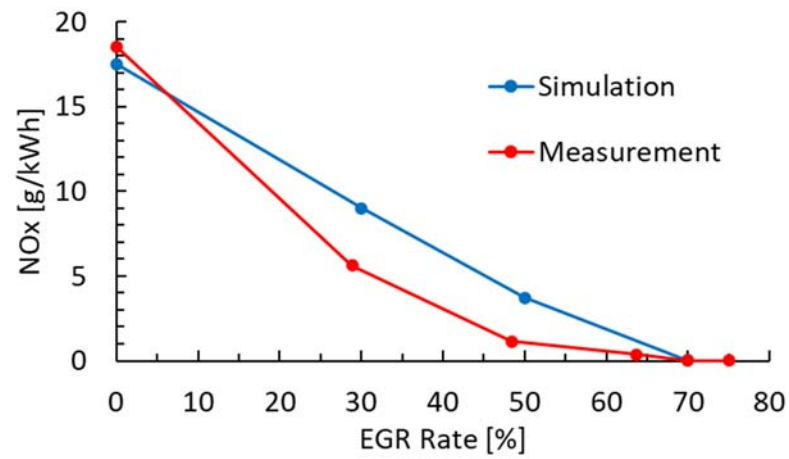
In addition, The PCCI simulations show that the AHRR in the combustion process has different peaks depending on the use of EGR. In the absence of EGR, there are two peaks in the heat release rate due to pilot and main injections. However, when using 30% EGR, the ignition delay is longer, resulting in the combination of heat rejection from the first and second injection event, leading to a higher peak in AHRR. When EGR is increased to 50-70%, auto-ignition is delayed by up to 7 °CA, resulting in a slower combustion process with a lower peak heat release rate.

As shown in **Figure 4.45**, NO_x, soot, and CO emission levels of various EGR rates for advanced split injection, simulations and experiments was compared. The results show that the calculated NO_x emissions for both the no-EGR and 70% EGR cases are aligned with the test results. However, for EGR rates of 30% and 50%, notable discrepancies between the CFD predictions and the empirical data were observed.

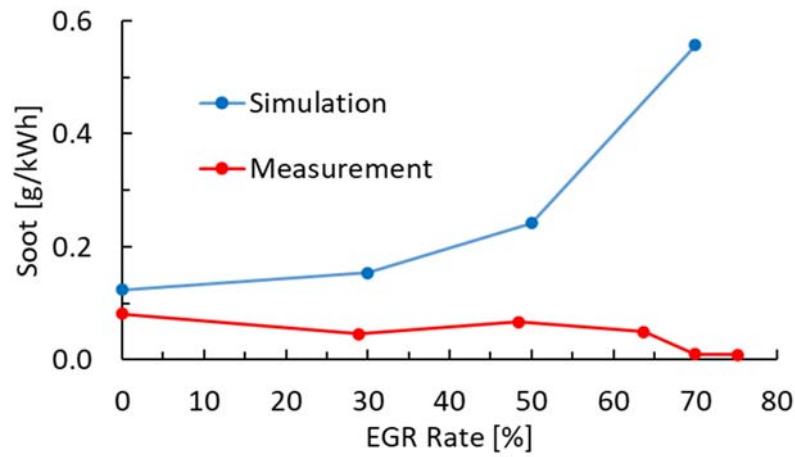
The prediction of soot emissions in the simulations relies on the Hiroyasu-NSC model, which is only partially empirical. However, the predicted figures do not match the actual results, and the disparity becomes greater as the EGR rate increases. To rectify this, the NSC soot oxidation model must be adjusted for low temperature oxidation to predict the accurate values of very advanced injection strategy of PCCI combustion under EGR operation.

CFD simulation accurately predicted CO emissions in the engine without EGR, but it was not as accurate for measurements with 30%, 50%, and 70% EGR rates. To improve accuracy, a more detailed kinetic mechanism is needed to model the low temperature combustion kinetics of CO oxidation under heavy EGR conditions.

a)



b)



c)

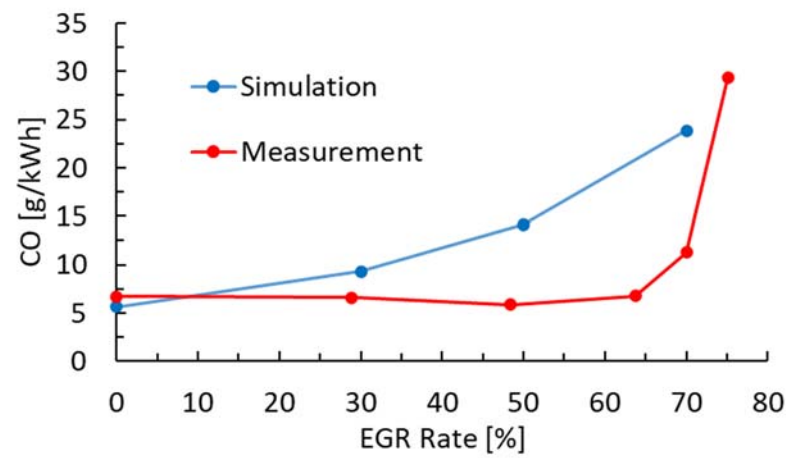


Figure 4.45: NO_x, soot and CO emission levels of various EGR rates for advanced split injection in the simulations and experiments.

4.7. Early Intake Valve Closing (EIVC) Cycle Analysis with Split Injection Strategy

The utilization of early intake valve closing strategy, also known as Miller cycle, has been suggested as a means of control the start and center of combustion (MFB50%) by reducing the effective compression ratio which enables a significant reduction of temperature and pressure levels before and during the combustion event of the combustion chamber.

Table 4.7 presents the effective compression ratios which is a ratio of actual volume during intake valve closing and top dead center of various intake valve closing event examined in this investigation.

Table 4.7: Effective compression ratio of the various intake valve closing events.

Effective Compression Ratio	
Base profile	17.10
40°CA EIVC	15.65
80°CA EIVC	13.73

Intake valve lift profiles used in this study are shown in **Figure 4.46**.

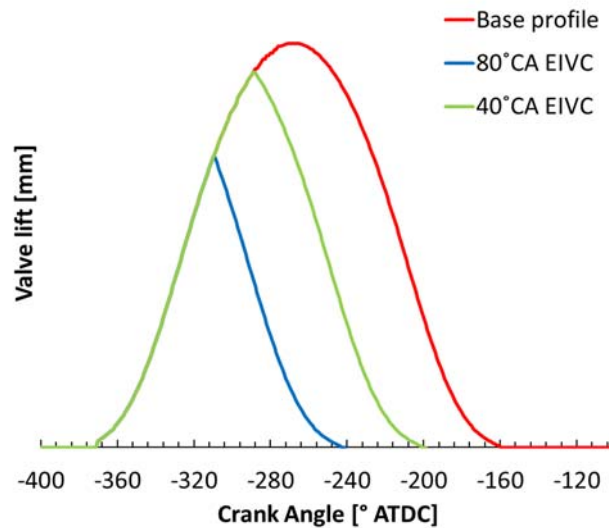


Figure 4.46: Intake valve lift profiles of various EIVC events.

The EIVC strategy reduces the amount of intake charge, which changes the way fuel is atomized, broken up, and evaporated in the engine. To prevent fuel spray from hitting the cylinder walls and to create a more uniform fuel-air mixture, a split injection strategy is used with EIVC. The charged mass in the EIVC events is reduced by up to

26% shown in **Table 4.8**. The intake valve closing profile shape effects the generation of swirl in the engine, and EIVC significantly reduces both amount of boosted air into the engine and swirl generation. Swirl ratio decreases more than 40%, in the intake valve closing. Swirl ratio history of various intake valve closing events are shown in **Figure 4.47**.

Table 4.8: Volumetric efficiency comparison of base and 40°CA and 80°CA EIVC events.

	Volumetric Efficiency [%]
Base profile	93.36
40°CA EIVC	81.68
80°CA EIVC	67.32

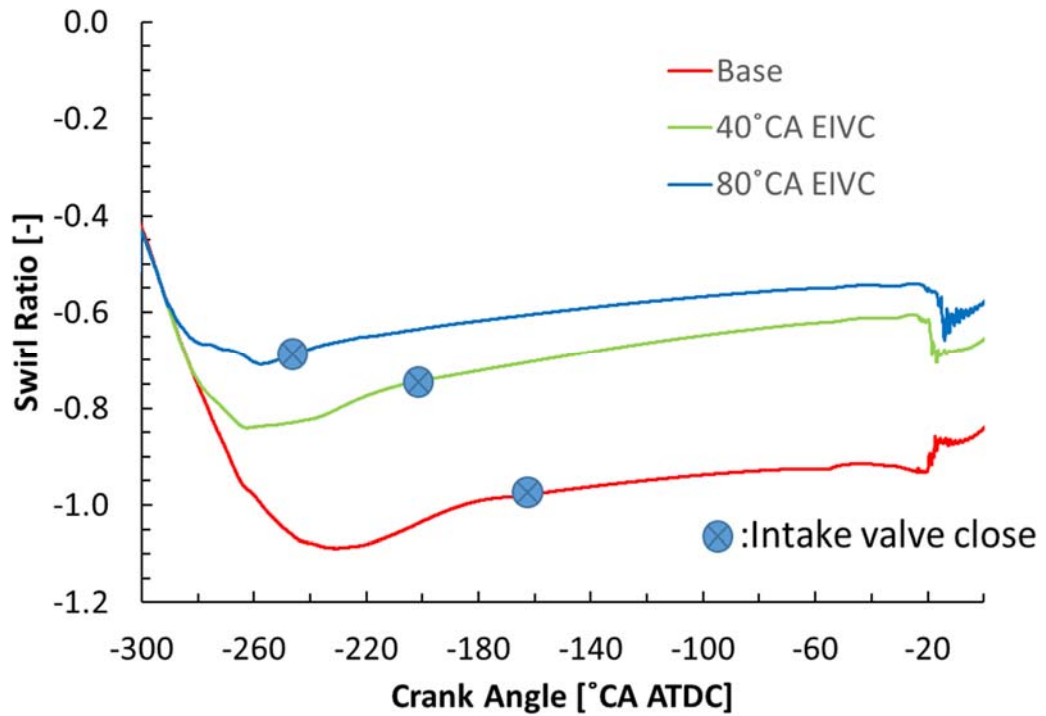


Figure 4.47: Swirl ratio history of various intake valve closing events.

The impact of engine early valve timing on in-cylinder fuel behavior can be seen in the fuel spray behavior. Specifically, reduction of in-cylinder pressure, temperature and density due to an EIVC profile effects fuel atomization quality, droplet break-up, and evaporation rate during the injection event. The study further examines the impact

of a split-injection with the first injection of SOI=-60 and second injection of SOI=-40°CA ATDC.

Liquid fuel mass in the combustion chamber is given in the **Figure 4.48** that, the base case exhibits higher evaporation rates of the liquid fuel, resulting in lower in-cylinder peak liquid masses after the pilot and main injections. As a result, the pilot injection is almost entirely evaporated by the start of the main injection, allowing for earlier completion of total fuel evaporation. However, in EIVC scenarios, the lower in-cylinder pressures and temperatures resulting from the reduced effective compression ratio cause almost one-third of the pilot injection to remain liquid form when the main injection starts. Compared to the base case, the evaporation of all injected fuel is consequently delayed.

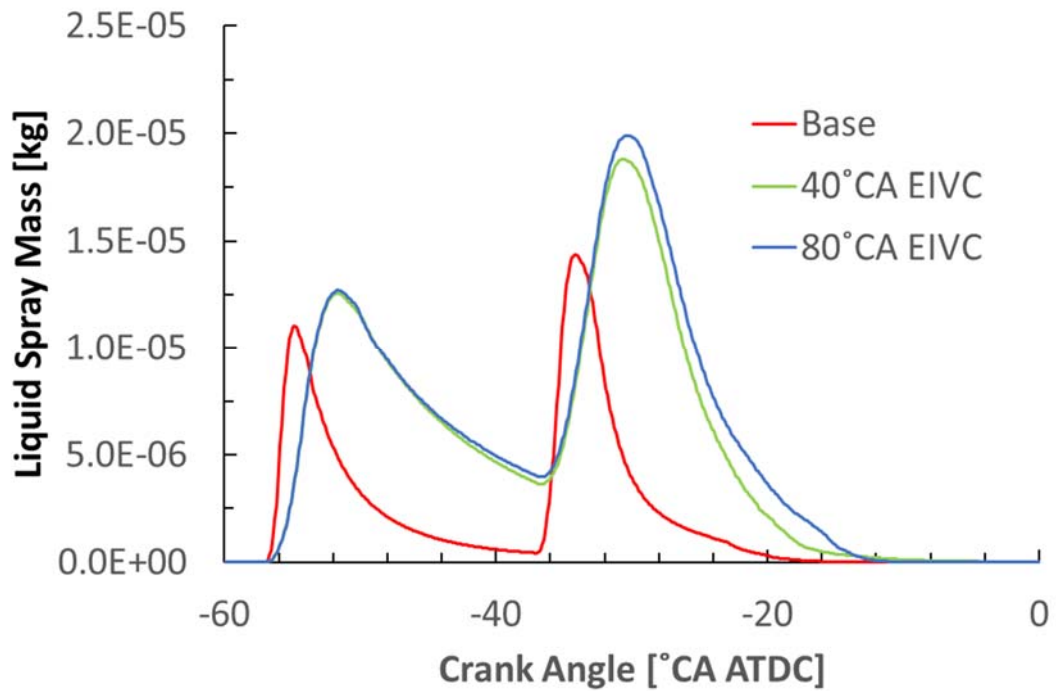


Figure 4.48: In-cylinder liquid fuel mass time histories for the base and 40 and 80 °CA EIVC cases.

Figure 4.49 shows the in-cylinder pressure and apparent HRR time histories observed of base and EIVC cam profile cases for various EGR rates ranging from 0% to 70%. In the no EGR case, the peak in-cylinder pressure experiences a reduction of 11 and 24 bars for the 40°CA and 80°CA EIVC profile cases, respectively, in comparison to

the base case. The EIVC profile cases exhibit a delay of 2 to 4°CA in the initiation of the first and primary combustion events. Additionally, the peak AHRR of the main combustion event due to premixed combustion increases from approximately 400J/°CA in the base case and 550J/°CA, 770J/°CA in the 40°CA and 80°CA EIVC cases, respectively. Moreover, in the EIVC cases, the center of combustion (CoC) approaches TDC by up to 4°CA. However, the end of combustion remains consistent across all cases.

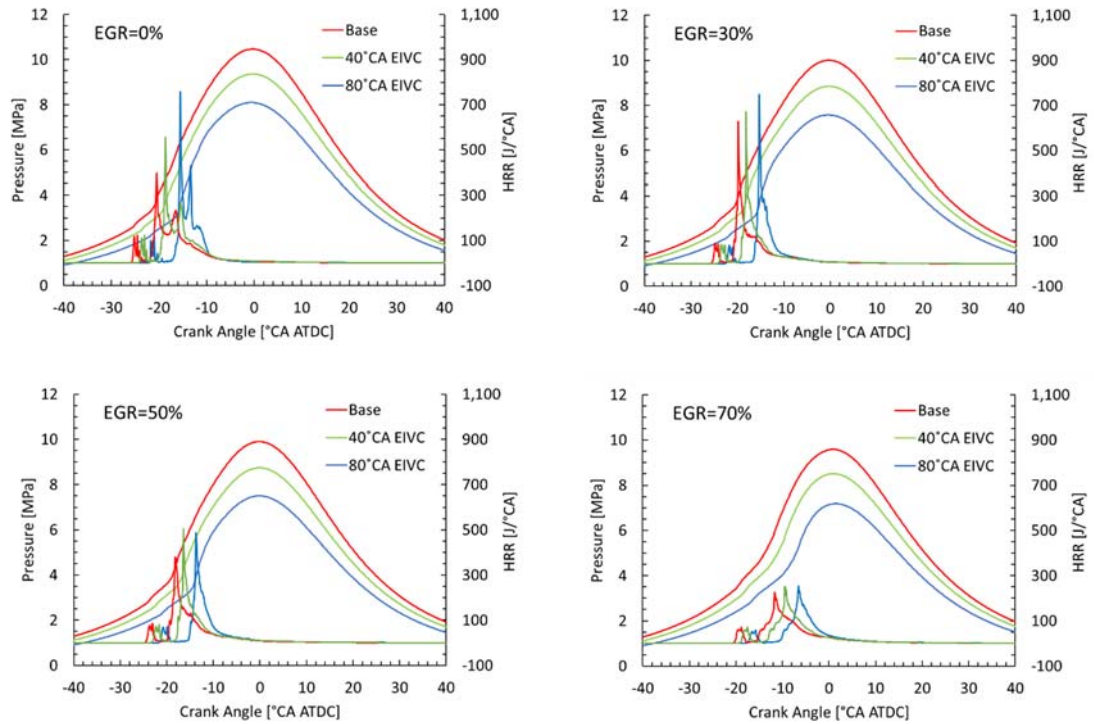


Figure 4.49: In-cylinder pressure and Apparent Heat Release Rate time histories of the base and EIVC profile cases for 0%, 30%, 50%, 70% EGR rates.

The results of the study show in

Figure 4.49 that in-cylinder pressure and apparent HRR time histories for various EGR rates exhibit distinct characteristics on combustion. Specifically, the SOI_{Ign} is not significantly effected by low and moderate EGR rates, but it is delayed by about 5°CA for a heavy EGR rate of 70%. Additionally, the peak apparent HRR of the main combustion event is reduced as the EGR rate increases, with a peak apparent HRR of less than 300J/°CA observed at a 70% EGR rate. Interestingly, there were not a

significant change in apparent HRR peak between the base and EIVC profile cases for heavy EGR rates.

The EIVC strategy is shown to have a significant effect on reduction of in-cylinder charge pressure and temperature by lowering the effective compression ratio. This delay in ignition and combustion is achieved by lower in-cylinder temperatures and pressures. The effects of EIVC profiles on the CoC for various EGR rates are illustrated in **Figure 4.50**. The delay in combustion, up to 4°CA, allows the CoC to approach TDC. Furthermore, the EGR ratio also plays a role in delaying the start of ignition and slowing the accumulation of heat release.

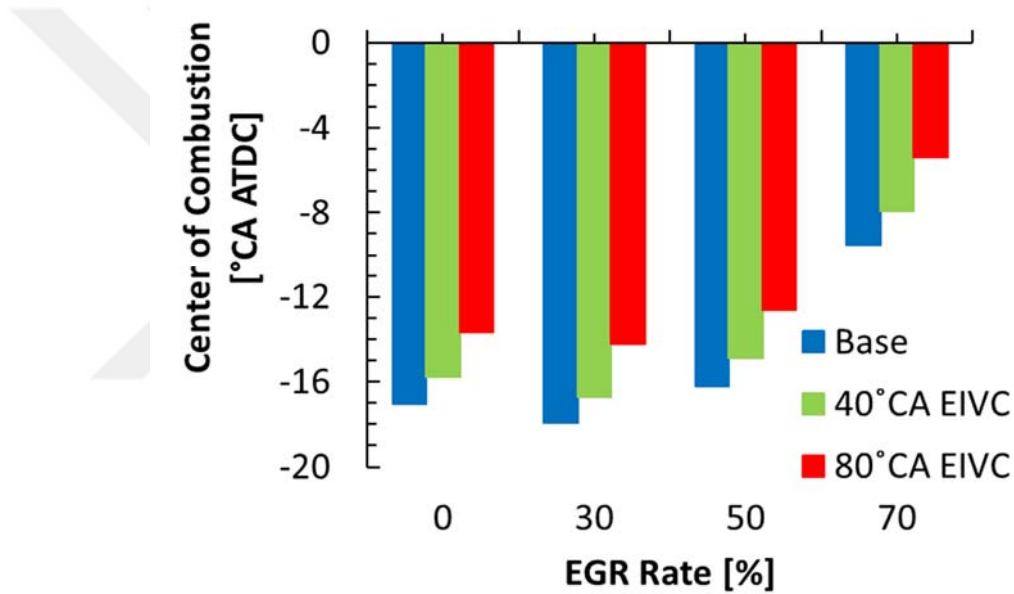


Figure 4.50: CoC (MFB50%) in the base and EIVC profile cases for various EGR rates.

The effect of EGR rate on combustion efficiency in the base and EIVC profile cases are shown in **Figure 4.51**. It is noted that the highest combustion efficiencies are achieved in the no EGR case, compared to EIVC cases. However, increasing the EGR rate leads to decreased combustion efficiency, with reductions of up to 4% and 5-8% for the base profile and EIVC profile cases, respectively. Reduction in O₂ concentration with EGR usage, significantly effects chemical kinetics and heat release rate during PCCI combustion following advanced injection. The author also highlights that EIVC cases experience a significant decrease in engine air charge capacity,

leading to a considerable reduction in combustion efficiency when combined with EGR and EIVC strategies.

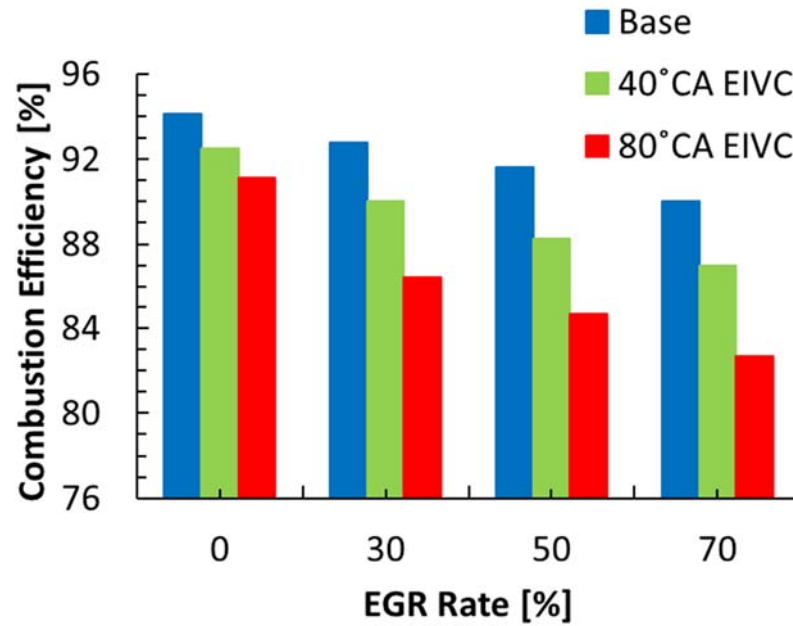


Figure 4.51: Combustion Efficiency of the base and EIVC profile cases for various EGR rates.

To better understand how heat is lost from the cylinder walls, heat transfer efficiency calculation is used. Heat transfer efficiency is the ratio of apparent accumulated heat release to the total heat released by chemical reactions energy in a cycle. In this study, it is evaluated engine heat transfer efficiency by calculating the ratio of apparent heat release based on pressure, volume, and polytropic coefficient time histories to the heat released by chemical reactions. Heat transfer efficiencies of the base and EIVC profiles at 0%, 30%, 50%, and 70% EGR rates are shown in **Figure 4.52**.

Under no EGR operation, there is more air in the combustion chamber during the base profile compared to when EIVC is used. This results in leaner combustion at lower temperatures and lower average gas temperatures during the expansion stroke, which improves heat transfer efficiency. However, when EGR is increased, the time it takes for the main combustion to start is longer. With heavy EGR and EIVC, the main combustion occurs closer to the TD, which improves the uniformity of the fuel vapor-air-gas mixture, resulting in a more uniform and slower main combustion, and thus, an increase in heat transfer efficiency.

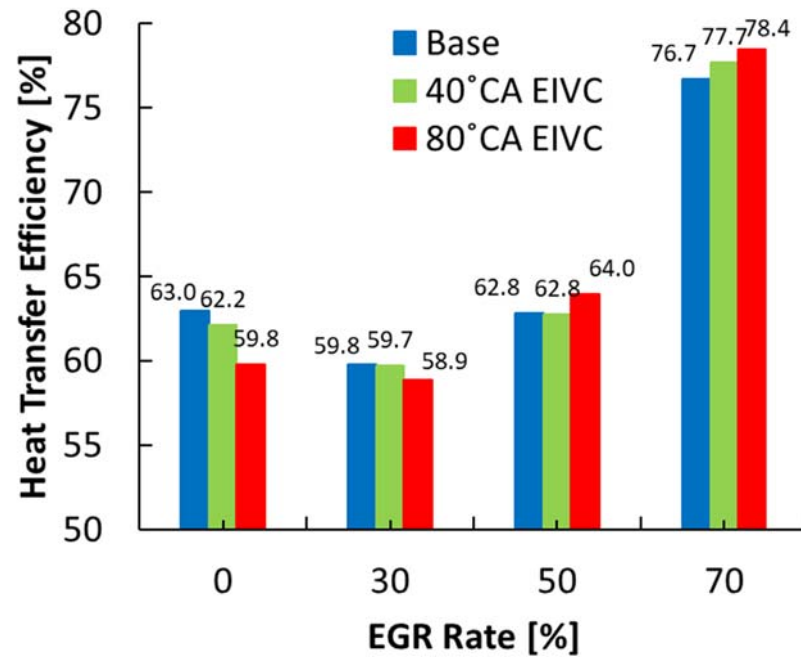


Figure 4.52: Heat transfer efficiency of the base and EIVC profile cases for various EGR rates.

Figure 4.53 displays the Indicated Specific Fuel Consumption data for the base and EIVC profile cases at varying EGR rates. Interestingly, the trend of ISFC in relation to EGR rate differs from that of combustion efficiency. The combination of combustion and heat transfer efficiencies, as well as the location of the CoC, determine the ISFC. In the case of a 30% EGR rate, combustion and heat transfer efficiencies decrease while the CoC advances, resulting in higher ISFC values. However, for a 70% EGR rate, an approximately 7.5°CA delayed CoC, along with elevated thermal efficiencies, lead to the best ISFC values for any IVC strategy, despite the deteriorated combustion efficiencies.

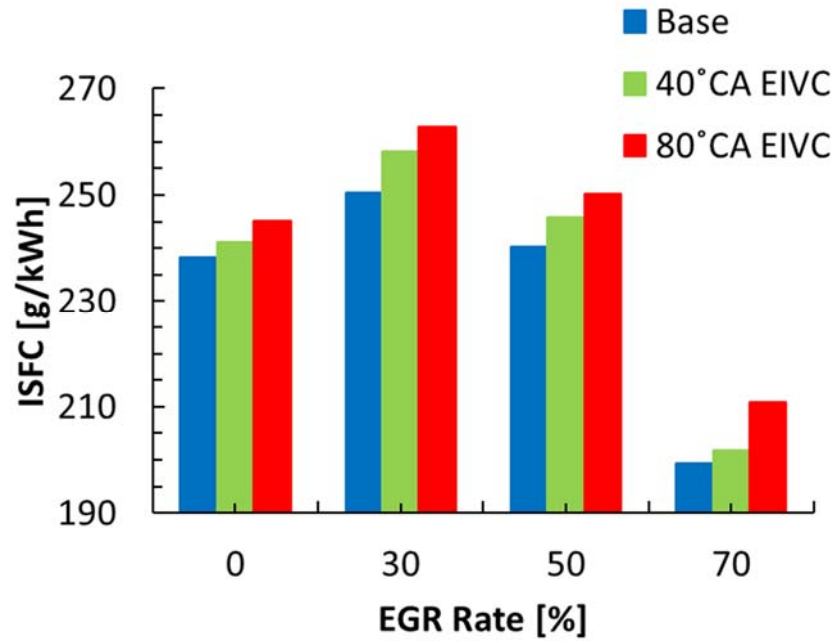


Figure 4.53: Indicated Specific Fuel Consumption of the base and EIVC profile cases for various EGR rates.

Figure 4.54 shows the NO_x emissions data for both the base and EIVC profile cases at various EGR rates. Higher EGR rates significantly reduce NO_x emissions, with extremely low NO_x emissions achieved in both the base and EIVC cases at a 70% EGR rate. A 30% EGR rate results in a 20% NO_x reduction for EIVC of 40°C. Minor changes in NO_x emissions occur between the base and EIVC profile cases for both the 50% and 70% EGR rates.

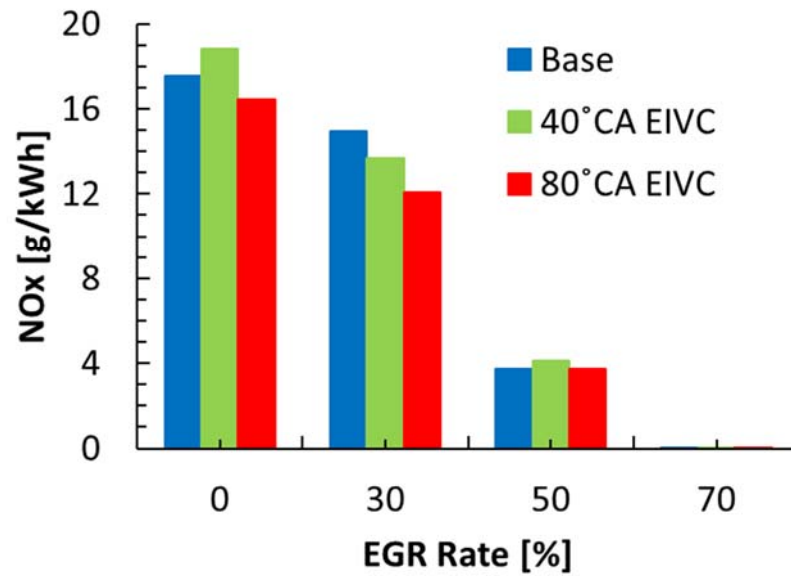


Figure 4.54: NO_x emissions of the base and EIVC profile cases for various EGR rates.

Figure 4.55 and **Figure 4.56** shows the soot and CO emissions for both the base and EIVC profile cases at EGR rates of 0%, 30%, 50%, and 70%. Soot emissions show a consistent increase until the 50% EGR rate, after which there is a significant increase in the soot levels. Similarly, the highest level of soot emissions is observed in the EIVC of 80°CA case, due to the lowest air to fuel ratio. On the other hand, CO emissions rise with the EGR rate due to incomplete combustion caused by lower O₂ concentration. The EIVC of 80°CA case yields the highest CO emissions, as the combustion efficiency values are the lowest, for any EGR rate.

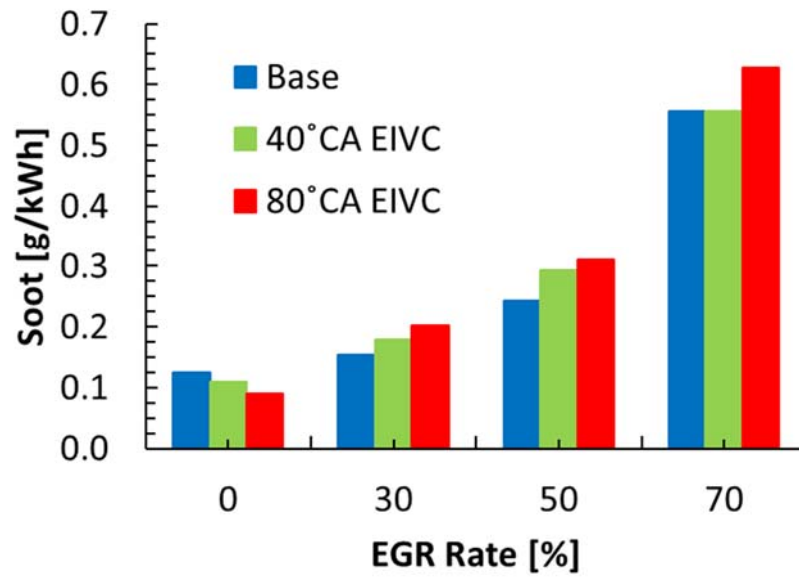


Figure 4.55: Soot emissions of the base and EIVC profile cases for various EGR rates.

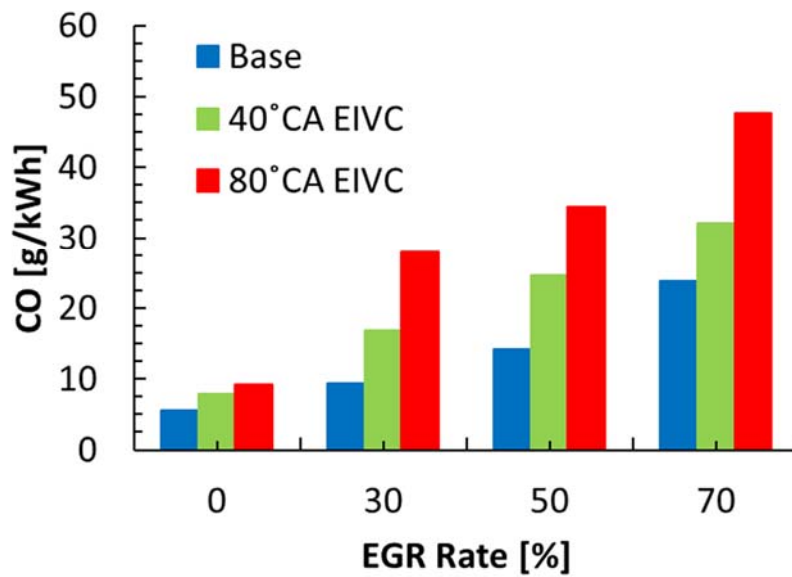


Figure 4.56: CO emissions of the base and EIVC profile cases for various EGR rates.

5. CONCLUSIONS

5.1. Experimental Study

In the experimental works performed in this project, the impact of injection timing and EGR rate on PCCI combustion characteristics and engine-out emissions for a single cylinder four stroke HDDI research engine operating at low load are investigated. Experimental tests for both single main injection strategy (SMIS) and split injection strategy (DIS) are conducted and measured heat release rate (HRR) and in-cylinder pressure (ICP) histories as well as ignition delay (ID), 50% mass fraction burn angle (MFB50%), indicated specific fuel consumption (ISFC), and engine-out emissions of NO_x, soot, unburned hydrocarbons (UHC) and carbon monoxide (CO). The experiments were performed under varying fuel rail pressures (FRP) of 800 bar, with SOI of SMIS and SPI of DIS varied between 70°CA and 0°CA before top dead center (BTDC), while SMI of DIS ranged between 50°CA and 0°CA BTDC, and EGR rate interval of 0% – 75%.

In summary, the timing of the start of injection (SOI) is crucial for achieving low engine-out NO_x emissions in SMIS-PCCI combustion. However, early SOI can lead to increased soot emissions due to spray impingement on cylinder walls. To reduce soot emissions, a 35% EGR rate can be used to shorten spray penetration. However, early SMIS can result in high ISFC, CO, and UHC emissions due to incomplete combustion of fuel wetting the cylinder walls.

A comparison of SMI, DIS, and TIS strategies reveals that the DIS strategy with an SPI-SMI pair of 60°CA and 40°CA BTDC, respectively, coupled with heavy EGR rates exceeding 45%, provides the lowest ISFC, soot, UHC, and CO emissions. This strategy is achieved by enhancing FVAM uniformity, preventing spray wall impingement, and leveraging low-temperature combustion, resulting in NO_x emissions below 2 g/kWh.

When using a diesel engine without exhaust gas recirculation (EGR), injecting one and two thirds of the fuel at specific points in the combustion cycle (SPI-SMI pairs of -60°CA & -50°CA and -50°CA & -45°CA after top dead center) can significantly reduce emissions of nitrogen oxides (NO_x) and soot compared to the base case with

no-EGR. However, fuel efficiency remains lower than the base case because the fuel injection occurs further away from top dead center. Additionally, incomplete combustion causes emissions of unburned hydrocarbons (UHC) to increase three to four times and carbon monoxide (CO) to increase drastically compared to the base case. Therefore, a diesel oxidation catalyst (DOC) is necessary to treat the UHC and CO emissions.

Utilizing early DIS-PCCI combustion with a SPI of 60 and SMI of 40 °CA before top dead center (BTDC), with a heavy exhaust gas recirculation (EGR) rate of 75.1%, we can achieve near zero NO_x emissions and a fuel consumption reduction of approximately 1% compared to the base CDC case. The heavy EGR rate reduces spray wall wetting and improves fuel-air mixing, leading to up to a 10% increase in (PCHTE at EGR rates above 40%. Additionally, the heavy EGR rate delays the start of ignition (SOIgn) and reduces the combustion speed, resulting in indicated mean effective pressure (IMEP) occurring closer to top dead center (TDC). Center of combustion of 20.3°CA BTDC for the no-EGR case to 6.7°CA BTDC for the 75.1% EGR rate leads to a 3.1% improvement in combustion conversion efficiency (CCE) and 4.6 g/kWh fuel savings compared to the base Diesel case.

To summarize, the implementation of PCCI strategy has challenge of wall wetting while achieving minimal engine-out NO_x emissions. An initial SMIS utilizing a traditional wide SIA injector and no/low-EGR results in spray wetting of the cylinder walls, leading to increased ISFC and engine-out emissions of soot, UHC, and CO. However, coupling DIS with high levels of EGR can diminish spray penetration, prevent wall wetting, enhance FVAM consistency, and delayed lean low temperature combustion towards TDC, resulting in engine-out NO_x and soot emissions close to zero with acceptable ISFC during partial load operation.

5.2. Computational Study of Injection Timing and SIA

In this section, computational study of injection timing and spray inclusion angle are investigated to gain a deeper understanding of the fuel spray and combustion phenomena associated with both conventional and advanced injection strategies. Through this research, it is explored how various spray inclusion angles impact the overall performance of these strategies and analyze the effects of different injection timings on combustion efficiency and spray wall interaction.

The impact of the timing of SOI and SIA on the combustion and emission traits of a single-cylinder HDDI diesel research engine for the PCCI combustion mode, using CFD simulations. The simulations were conducted on a comprehensive 3D CFD model of a full-cycle, with a simplified chemical kinetic mechanism of n-heptane surrogate fuel, at 1100 rpm engine speed and 3-bar IMEP operating conditions.

It has been observed that the Hiroyasu-NSC semi-empirical model predicted a significantly higher value of soot emissions in the PCCI combustion case, approximately two times higher than the actual measured value. To address this discrepancy, it is recommended to calibrate the Arrhenius pre-exponential factor for soot-formation kinetics (A_{sf}) and the scaling factor of NSC soot oxidation model (A_{so}) in the soot-formation and oxidation rate equations, respectively, based on temperature. This would enable the development of a unified formulation that accounts for both diffusion-controlled and PCCI combustion.

For an SIA of 146, delaying SOI results the fuel spray penetration rate and peak liquid fuel mass in the cylinder to decrease. By varying the SOI between -70° and -10° CA ATDC, the ID decreases from 44.2 to 4.1 degrees CA, while the combustion efficiency and IMEP increase from 58.5% to 99.9% and 1.99 to 3.89 bar, respectively. The highest and lowest pressure peaks inside the cylinder are obtained for SOI timings of -30° and -70° CA ATDC, with peaks of 10.1 MPa and 8.8 MPa, respectively.

To achieve diffusion-controlled combustion, an SIA of 146° is required in delayed injection cases where the SOI is after -30° CA ATDC. For optimal results, an SOI of -10° CA ATDC is recommended, which yields complete diffusion-controlled combustion and impressive CE and IMEP of 99.9% and 3.89 bars, respectively. Additionally, engine-out soot and CO emissions are reduced to a minimum of 17 ppm and 16 ppm, respectively. However, this comes at the cost of higher NO_x emissions of 1136.7 ppm due to increased flame temperatures compared to PCCI combustion cases.

Using an SIA of 146° , in the early injection cases with SOI timings of -50° CA ATDC and -70° CA ATDC, PCCI combustion IDs occur at 24.7° CA and 44.2° CA, respectively. These values are significantly higher than those of CDC, which range between 4.1° CA and 8.4° CA depending on the SOI. In diffusion-controlled combustion, NO_x emissions are 1336.7 ppm, 2368.6 ppm, and 3533.3 ppm for SOI timings of -10° , -20° , and -30° CA ATDC, respectively. However, PCCI cases with

SOI timings of $-50^{\circ}\text{CA ATDC}$ and $-70^{\circ}\text{CA ATDC}$ result in significantly decreased NO_x emissions of 54.8 ppm and 4.04 ppm, respectively, due to low-temperature combustion.

In PCCI combustion, soot emissions of 147.8 ppm and 206.8 ppm for SOI timings of -70 and $-50^{\circ}\text{CA ATDC}$, respectively, are significantly higher than those of diffusion-controlled combustion due to persistent soot production caused by wall-wetting and insignificant soot oxidation rates at lower in-cylinder temperatures. Despite lower CO production rates in PCCI combustion, engine-out CO emission is 648.9 ppm for SOI timings of $-70^{\circ}\text{CA ATDC}$ and 935.0 ppm for SOI timings of $-50^{\circ}\text{CA ATDC}$, which are significantly higher as compared to those for diffusion-controlled combustion.

In an ESI with an SOI of $-50^{\circ}\text{CA ATDC}$, the SIA sweep showed that using an injector with a narrow SIA of 100° led to the best results. This was due to high-temperature lean-premixed combustion of well-mixed FVAM. The highest CE of 97.8%, and the lowest soot and CO emissions of 33.5 ppm and 2.2 ppm, respectively, and IMEP of 3.37 bars were achieved. Additionally, acceptable NO_x emissions of 6.5×10^{-6} kg/stroke were observed. To achieve these results, the spray was targeted to the tip of the stepped lip of the piston bowl, resulting in a lean mixture in most of the combustion chamber. A slightly rich mixture was spread within the piston bowl, in the squish region and beneath the valves.

The effect of spray angle (SIA) on mixture formation, combustion, and emissions in a diesel engine is investigated. The engine is operated with an SOI of $-50^{\circ}\text{CA ATDC}$, and four different SIAs (146° , 140° , 130° , and 120°) are used. Results show that the spray with an SIA of 140° leads to poor mixture formation, resulting in the lowest CE and the smallest IMEP. On the other hand, the highest soot and CO emissions are observed for an SIA of 130° and 140° . However, the 140° SIA also exhibits near-zero NO_x emissions due to low-temperature combustion of a poor-quality fuel-air mixture. These findings suggest that the selection of spray angle can significantly effect engine performance and emissions, and further optimization is required to achieve the desired balance between efficiency and emissions.

To sum up, it can be stated that the attainment of optimum combustion efficiency and minimized engine-out emissions across all operational conditions can be effectively accomplished through the utilization of a fuel-injection system that is equipped with

an adaptive control mechanism for SIA which is synchronized with the injection timing(s) that are necessitated by the engine load.

5.3. Computational Study of EIVC

In this section, a comprehensive 3D computational fluid dynamics simulations are used to investigate the impact of EGR rate and a highly advanced split injection technique on PCCI combustion and engine-out emissions in a HDDI diesel engine operating under part load condition with EIVC strategy.

It has been found that a split injection strategy is to be particularly effective in advanced injection strategy of PCCI combustion. By splitting the injection, the fuel can be more effectively distributed throughout the combustion chamber and reducing spray wall wetting, leading to improved fuel efficiency and reduced emissions. Additionally, this approach can help to minimize the formation of harmful pollutants such as NO_x and particulate matter. Overall, the use of a split injection strategy represents an important tool for optimizing engine performance and meeting increasingly stringent emissions regulations.

It was observed that the implementation of an EIVC strategy resulted in delayed combustion events and decreased combustion efficiency in both non-EGR and up to 70% EGR rate operating conditions. The ISFC of the engine was also found to be higher in the EIVC strategy compared to the base IVC case, irrespective of the EGR rate. However, the use of an EIVC profile of 80° CA at no-EGR and 30% EGR rate resulted in decreased NO_x emissions compared to the baseline and an EIVC profile of 40° CA. It was also observed that soot emissions increased significantly with EGR rate, while the increase in soot emissions due to EIVC profiles was relatively small. On the other hand, CO emissions gradually increased with the EGR rate, but the EIVC strategy significantly increased CO emissions due to incomplete combustion caused by insufficient mixing of fuel vapor with air.

The Miller cycle is known to have a negative impact on various aspects of engine performance and emissions. Specifically, it can lead to poor fuel atomization and mixture formation, incomplete combustion, elevated soot formation, and increased CO emissions. These adverse effects are largely due to the lower pressure environment and reduced swirl associated with the Miller cycle. To mitigate these issues, future

research may focus on implementing a late IVC strategy, early split injection, and heavy EGR. By doing so, it may be possible to optimize engine performance and minimize the negative effects of the Miller cycle.

5.4. Future Works

In this thesis, the impact of injection strategy, timing, and EGR rate on the performance and emissions of a single-cylinder HDDI Diesel engine operating in PCCI combustion mode at low load was examined through experimental analysis, without making any changes to the engine hardware. It is found that, early DIS-heavy EGR rate is very effective to control NO_x , soot emissions, to reduce the spray wall impingement while similar even better fuel consumption at part load engine operation.

At cold-start and warm-up, incomplete combustion can lead to high engine-out UHC, CO, and NO_x emissions due to poor fuel atomization and evaporation, as well as fuel film formation on cylinder walls after late DIS. By implementing an early DIS-heavy EGR rate strategy, fuel evaporation and FVAM formation can be improved, reducing emissions [151], [152]. However, to accelerate DOC and SCR light-off times and meet future tailpipe-out emissions regulations, a combination of strategies such as intake air throttling or heating, high-temperature glow plugs with temperature control, additional vaporized Diesel fuel injection before DOC, improved DPF catalyst, enhanced small low temperature close-coupled LNT, and suitably configured electrically heated catalysts with thermal management is necessary [153], [154]. Further research is required to explore the effects of early DIS-heavy EGR rate combined with intake air heating and high-temperature glow plug strategy on combustion and engine-out emissions at cold-start and warm-up.

To expand the load range of PCCI combustion, computational investigations are performed of various factors such as SIA, CR, and Miller cycles, with the aim of enhancing fuel air mixing and thermal efficiency while simultaneously decreasing spray wall wetting, soot, NO_x , and UHC emissions. Further investigation will be explored the potential impact of implementing cylinder charge active temperature and swirl control, variable compression ratio into the diesel engine on early DIS-heavy EGR rate operation. ref ver. [96], [155], [156], [157], [158].

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BIOGRAPHY

Cengizhan Cengiz, completed his undergraduate studies in Mechanical Engineering at Istanbul Technical University in 2006. He gets a master's degree in Aeronautics and Astronautics Faculty in Istanbul Technical University in 2009, where he also worked as a Research Assistant on a Tubitak 106M228 “Use of ILDM and CFD methodologies for Reducing Emissions from Diesel Engines” Project. In 2009, he joined Ford Otosan A.Ş Product Development Center as a CFD engineer, and later worked as a Calibration Engineer at the Calibration and Control Department until 2019. Currently, Cengiz is working as a Combustion Technical Leader in Ford Otosan. He has been started his doctorate studies in Mechanical Engineering at Gebze Technical University since 2016. His professional interests include internal combustion engine combustion, alternative fuel modes, thermodynamic analysis of internal combustion engines, engine design, combustion chamber design, port development, measurement systems, racing engines, and calibration and control. He is also leading the operation of single cylinder research and hydrogen engines.

PUBLICATIONS AND PRESENTATIONS FROM THE THESIS

[1] Cengiz, C., Unverdi, S.O., (2023), “A CFD Study on the Effects of Injection Timing and Spray Inclusion Angle on Performance and Emission Characteristics of a DI Diesel Engine Operating in Diffusion-Controlled and PCCI Modes of Combustion”, *Energies*, 16 (6), 2861. <https://doi.org/10.3390/en16062861>

[2] Cengiz, C., Unverdi, S.O., (2023), “Effect of early intake valve closing, exhaust gas recirculation and split injection on combustion and emissions characteristics of a HDDI diesel engine operating in PCCI combustion mode”, *Fuel*, 353. <https://doi.org/10.1016/j.fuel.2023.129079>

[3] Cengiz, C., Unverdi, S.O., (2022), “Investigation of Early Intake Valve Closing Strategy and Exhaust Gas Recirculation (EGR) on PCCI Engine Operation”, 16th International Combustion Symposium, 1-8, Aydın, Türkiye, 8-11 September.

APPENDICES

APPENDIX-A: REACTION MECHANISM USED IN THE SIMULATIONS

elements

h c o n
end

specie

c7h16 o2 n2 co2 h2o
co h2 ch4 c2h2 c2h4
h2o2 ho2 oh
h o
ch3 ch3o
ch2 ch2o ch3o2 ch4o2 hco
c7h15-1 c7h15-2 c7h15o2 c7h14o2h c7h14o2ho2 c7ket12
c6h12 c5h11cho c5h11co c5h11 c4h9
c3h7 c3h6 c3h5 c3h4
c2h3 c2h5 c2h6
!ch3hco ch3co hcooch3 cooch3
!n2o no n
no n
end

reactions

c7h16 + h	= c7h15-1 + h2	5.600e+07	2.0	7667.0!
c7h16 + h	= c7h15-2 + h2	4.380e+07	2.0	4750.0!
c7h16 + oh	= c7h15-1 + h2o	8.610e+09	1.10	1815.0!
c7h16 + oh	= c7h15-2 + h2o	4.500e+09	1.30	690.5!
c7h16 + ho2	= c7h15-1 + h2o2	1.120e+13	0.0	19300.0!
c7h16 + ho2	= c7h15-2 + h2o2	1.650e+13	0.0	16950.0!
c7h16 + o2	= c7h15-1 + ho2	2.500e+13	0.0	48810.0!
c7h16 + o2	= c7h15-2 + ho2	2.000e+14	0.0	47380.0!

c7h15-1 + o2	= c7h15o2	2.000e+12	0.0	0.0!	
c7h15-2 + o2	= c7h15o2	2.000e+12	0.0	0.0!	
c7h15o2	= c7h14o2h	6.000e+11	0.0	20380.0!	
c7h14o2h + o2	= c7h14o2ho2	4.600e+11	0.0	0.0!	
c7h14o2ho2	= c7ket12 + oh	1.000e+09	0.0	7480.0!	
c7ket12	= c5h11cho + ch2o + o	1.050e+16	0.0	4.110e+4!	16
c5h11cho + o2	= c5h11co + ho2	2.000e+13	0.5	4.220e+4!	
c5h11cho + oh	= c5h11co + h2o	1.000e+13	0.0	0.000e+0!	
c5h11cho + h	= c5h11co + h2	4.000e+13	0.0	4.200e+3!	
c5h11cho + o	= c5h11co + oh	5.000e+12	0.0	1.790e+3!	
c5h11cho + ho2	= c5h11co + h2o2	2.800e+12	0.0	1.360e+4!	
c5h11cho + ch3	= c5h11co + ch4	1.700e+12	0.0	8.440e+3!	
c5h11cho + ch3o2	= c5h11co + ch4o2	1.000e+12	0.0	9.500e+3!	
c5h11co	= c5h11 + co	1.000e+11	0.0	9.600e+3!	
c5h11	= c2h4 + c3h7	3.200e+13	0.0	28300.0!	
c7h15-1	= c2h4 + c5h11	2.500e+13	0.0	28810.0!	
c7h15-2	= c4h9 + c3h6	2.200e+13	0.0	28100.0!	
c7h15-1	= c7h15-2	3.600e+16	0.0	80700.0!	
c4h9	= c2h5 + c2h4	2.500e+13	0.0	28810.0!	
c3h7	= c2h4 + ch3	9.600e+13	0.0	30950.0!	
c3h7	= c3h6 + h	1.250e+14	0.0	36900.0!	
c3h7 + o2	= c3h6 + ho2	1.000e+12	0.0	4980.0!	
c3h6	= c2h3 + ch3	3.150e+15	0.0	85500.0!	
c3h6 + h	= c3h5 + h2	5.000e+12	0.0	1500.0!	
c3h6 + ch3	= c3h5 + ch4	9.000e+12	0.0	8480.0!	
c3h5	= c3h4 + h	4.000e+13	0.0	69760.0!	
c3h5 + h	= c3h4 + h2	1.000e+13	0.0	0.0!	
c3h5 + o2	= c3h4 + ho2	6.000e+11	0.0	10000.0!	
c3h4 + oh	= c2h3 + ch2o	1.000e+12	0.0	0.0!	
c3h4 + oh	= c2h4 + hco	1.000e+12	0.0	0.0!	
!					
!c2h5 + o	= ch3hco + h	5.300e+13	0.0	0.0!	23
!c2h4 + ho2	= hcooch3 + h	4.040e+09	0.0	-840.!	24
!c2h4 + ho2	= ch3hco + oh	2.200e+13	0.0	17200.0!	25

$\text{!c2h4} + \text{ch3o} = \text{ch3hco} + \text{ch3} \quad 3.000\text{e}+13 \quad 0.0 \quad 14500.0 \quad ! \quad 26$
 $\text{!c2h4} + \text{ch3o2} = \text{ch3hco} + \text{ch3o} \quad 7.000\text{e}+13 \quad 0.0 \quad 14500.0 \quad ! \quad 27$
 $\text{!c2h3} + \text{oh} = \text{ch3hco} \quad 3.000\text{e}+13 \quad 0.0 \quad 0.0! \quad 28$
 !
 $\text{!ch3hco} = \text{ch3} + \text{hco} \quad 7.080\text{e}+15 \quad 0.00 \quad 81760.! \quad 28$
 $\text{!ch3hco} = \text{ch3co} + \text{h} \quad 5.000\text{e}+14 \quad 0.00 \quad 87860.! \quad 29$
 $\text{!ch3hco} + \text{o2} = \text{ch3co} + \text{ho2} \quad 2.000\text{e}+13 \quad 0.50 \quad 42200.! \quad 30$
 $\text{!ch3hco} + \text{h} = \text{ch3co} + \text{h2} \quad 4.100\text{e}+13 \quad 0.00 \quad 4200.! \quad 31$
 $\text{!ch3hco} + \text{oh} = \text{ch3co} + \text{h2o} \quad 1.000\text{e}+13 \quad 0.00 \quad 0.! \quad 32$
 $\text{!ch3hco} + \text{o} = \text{ch3co} + \text{oh} \quad 5.800\text{e}+12 \quad 0.00 \quad 1790.! \quad 33$
 $\text{!ch3hco} + \text{ch3} = \text{ch3co} + \text{ch4} \quad 1.700\text{e}+12 \quad 0.0 \quad 8440.0! \quad 34$
 $\text{!ch3hco} + \text{ch2} = \text{ch3co} + \text{ch3} \quad 1.660\text{e}+12 \quad 0.0 \quad 3510.! \quad 35$
 $\text{!ch3hco} + \text{ho2} = \text{ch3co} + \text{h2o2} \quad 1.700\text{e}+12 \quad 0.00 \quad 10700.! \quad 36$
 $\text{!ch3hco} + \text{ch3o2} = \text{ch3co} + \text{ch4o2} \quad 1.150\text{e}+11 \quad 0.0 \quad 10000.0! \quad 37$
 $\text{!ch3co} + \text{o} = \text{ch3} + \text{co2} \quad 1.000\text{e}+13 \quad 0.00 \quad 0.! \quad 38$
 $\text{!ch3co} + \text{h} = \text{ch3} + \text{hco} \quad 1.000\text{e}+14 \quad 0.0 \quad 0.! \quad 39$
 $\text{!ch3co} + \text{oh} = \text{ch3} + \text{co} + \text{oh} \quad 3.000\text{e}+13 \quad 0.0 \quad 0.! \quad 40$
 $\text{!ch3co} + \text{ho2} = \text{ch3} + \text{co2} + \text{oh} \quad 3.000\text{e}+13 \quad 0.0 \quad 0.! \quad 42$
 $\text{!ch3co} + \text{ch3} = \text{c2h6} + \text{co} \quad 5.000\text{e}+13 \quad 0.00 \quad 0.! \quad 43$
 !
 $\text{!hcooch3} = \text{hco} + \text{ch3o} \quad 3.200\text{e}+09 \quad 1.60 \quad 51800.! \quad 44$
 $\text{!hcooch3} = \text{co2} + \text{ch4} \quad 2.950\text{e}+09 \quad 0.00 \quad 24500.! \quad 45$
 $\text{!hcooch3} + \text{o} = \text{cooch3} + \text{oh} \quad 5.300\text{e}+11 \quad 0.60 \quad 1470.! \quad 46$
 $\text{!hcooch3} + \text{h} = \text{cooch3} + \text{h2} \quad 1.600\text{e}+08 \quad 1.60 \quad 1000.! \quad 47$
 $\text{!hcooch3} + \text{oh} = \text{cooch3} + \text{h2o} \quad 1.200\text{e}+09 \quad 1.30 \quad -150.! \quad 48$
 $\text{!hcooch3} + \text{ho2} = \text{cooch3} + \text{h2o2} \quad 4.000\text{e}+12 \quad 0.00 \quad 6100.! \quad 49$
 $\text{!hcooch3} + \text{ch3} = \text{cooch3} + \text{ch4} \quad 1.000\text{e}-02 \quad 4.50 \quad 1800.! \quad 50$
 $\text{!cooch3} = \text{ch3} + \text{co2} \quad 8.730\text{e}+42 \quad -8.62 \quad 22400.! \quad 51$
 !
 $\text{ch3o} + \text{co} = \text{ch3} + \text{co2} \quad 1.570\text{e}+14 \quad 0.00 \quad 11800.! \text{!cgs} \quad 52$
 $\text{ch3o} + \text{m} = \text{ch2o} + \text{h} + \text{m} \quad 1.000\text{e}+14 \quad 0.00 \quad 25000.! \text{!cgs} \quad 53$
 $\text{ch3o} + \text{h} = \text{ch2o} + \text{h2} \quad 2.000\text{e}+13 \quad 0.00 \quad 0.! \text{!cgs} \quad 54$
 $\text{ch3o} + \text{oh} = \text{ch2o} + \text{h2o} \quad 1.000\text{e}+13 \quad 0.00 \quad 0.! \text{!cgs} \quad 55$
 $\text{ch3o} + \text{o} = \text{ch2o} + \text{oh} \quad 1.000\text{e}+13 \quad 0.00 \quad 0.! \text{!cgs} \quad 56$

ch3o + o2	= ch2o + ho2	1.200e+11 0.00 2600. !cgs 57 10
ch3 + ho2	= ch3o + oh	5.000e+13 0.00 0. !cgs 58
ch3 + o2	= ch3o + o	4.670e+13 0.00 30000. !cgs 59
ch3 + o2	= ch2o + oh	3.800e+11 0.00 9000. !cgs 60 4.8 9000
ch3 + o2	= ch3o2	3.020e+59 -15.0 17204. !cgs 61 3.02
ch3o2 + ho2	= ch4o2 + o2	4.630e+11 0.0 -2583. !cgs 24
ch3o2 + ch4	= ch4o2 + ch3	1.810e+11 0.0 18480. !cgs 25
ch3o2 + ch3	= ch3o + ch3o	2.410e+13 0.0 0. !cgs 26 2.410e+13
ch3o2 + o	= ch3o + o2	3.610e+13 0.0 0. !cgs 27
ch3o2 + h	= ch3o + oh	9.640e+13 0.0 0. !cgs 28
ch3o2 + ch2o	= ch4o2 + hco	1.000e+12 0.0 11665. !cgs 29
ch3o2 + c2h6	= ch4o2 + c2h5	2.950e+11 0.0 14944. !cgs 30
ch3o2 + ch3o2	= ch3o + ch3o + o2	2.800e+11 0.0 -780. !cgs 31 11
ch3o2 + h2o2	= ch4o2 + ho2	2.400e+12 0.0 10000. !cgs 32
ch4o2	= ch3o + oh	3.000e+16 0.0 42920. !cgs 33 6.000e+16
ch3o2 + c2h4	= c2h3 + ch4o2	7.100e+11 0.0 17110. !cgs 34
ch4o2 + oh	= ch3o2 + h2o	1.000e+13 0.0 -258. !cgs 35 ! 8.2
ch4o2 + o	= ch3o2 + oh	2.000e+13 0.0 4750. !
ch3 + o	= ch2o + h	8.000e+13 0.00 0. !cgs 36
ch3 + oh	= ch2 + h2o	7.500e+06 2.00 5000. !cgs 37
ch3 + oh	= ch2o + h2	4.000e+12 0.00 0. !cgs 38
ch3o + h	= ch3 + oh	1.000e+14 0.00 0. !cgs 39
co + o + m	= co2 + m	6.170e+14 0.00 3000. !cgs 40
co + oh	= co2 + h	3.510e+07 1.30 -758. !cgs 41
co + o2	= co2 + o	1.600e+13 0.00 41000. !cgs 42
ho2 + co	= co2 + oh	5.800e+13 0.00 22930. !cgs 43
!		
h2 + o2	= oh + oh	1.700e+13 0.00 47780. !cgs 44
h2 + oh	= h2o + h	1.170e+09 1.30 3626. !cgs 45
o + oh	= o2 + h	4.000e+14 -0.50 0. !cgs 46
o + h2	= oh + h	5.060e+04 2.67 6290. !cgs 47
h + ho2	= o + h2o	3.100e+10 0.00 3590. !cgs 48
o + oh + m	= ho2 + m	1.000e+16 0.00 0. !cgs 49
h2o/21./ co2/5.0/ h2/3.3/ co/2.0/		

h + o2 + m = ho2 + m	3.600e+17 -0.72	0. !cgs 50
h2o/21./ co2/5.0/ h2/3.3/ co/2.0/		
oh + ho2 = h2o + o2	7.500e+12 0.00	0. !cgs 51
h + ho2 = oh + oh	1.700e+14 0.0	875. !cgs 52
o + ho2 = o2 + oh	1.400e+13 0.00	1073. !cgs 53
oh + oh = o + h2o	6.000e+08 1.30	0. !cgs 54
h + h + m = h2 + m	1.000e+18 -1.00	0. !cgs 55
h2/0./ h2o/0./ co2/0./		
h + h + h2 = h2 + h2	9.200e+16 -0.60	0. !cgs 56
h + h + h2o = h2 + h2o	6.000e+19 -1.25	0. !cgs 57
h + h + co2 = h2 + co2	5.490e+20 -2.00	0. !cgs 58
h + oh + m = h2o + m	1.600e+22 -2.00	0. !cgs 59
h + o + m = oh + m	6.200e+16 -0.60	0. !cgs 60
o + o + m = o2 + m	1.890e+13 0.00	-1788. !cgs 61
h + ho2 = h2 + o2	1.250e+13 0.00	0. !cgs 62
ho2 + ho2 = h2o2 + o2	2.000e+12 0.00	0. !cgs 63
h2o2 + m = oh + oh + m	4.300e+16 0.00	45500. !cgs 64
h2o/21./ co2/5.0/ h2/3.3/ co/2.0/		
h2o2 + h = ho2 + h2	1.600e+12 0.00	3800. !cgs 65
h2o2 + oh = h2o + ho2	1.000e+13 0.00	1800. !cgs 66
h2o2 + h = h2o + oh	1.000e+13 0.00	3590. !cgs
h2o2 + o = h2o + o2	8.400e+11 0.00	4260. !cgs
h2o2 + o = oh + ho2	2.000e+13 0.00	5900. !cgs
h2 + ho2 = h2o + oh	6.500e+11 0.00	18800. !cgs
!		
!co2 + n = no + co	1.900e+11 0.00	3400. !cgs 67
!n2o + o = n2 + o2	1.400e+12 0.00	10810. !cgs 68
!n2o + o = no + no	2.900e+13 0.00	23150. !cgs 69
!n2o + h = n2 + oh	4.400e+14 0.00	18880. !cgs 70
!n2o + oh = n2 + ho2	2.000e+12 0.00	21060. !cgs
!n2o + m = n2 + o + m	1.300e+11 0.00	59620. !cgs
n + no = n2 + o	3.270e+12 0.30	0. !cgs
n + o2 = no + o	6.400e+09 1.00	6280. !cgs
n + oh = no + h	7.333e+13 0.00	1120. !cgs

!

ch2o + o2	= hco + ho2	6.200e+13	0.00	39000. !cgs	
ch2o + o	= hco + oh	1.800e+13	0.00	3080. !cgs	
ch2o + h	= hco + h2	2.190e+08	1.80	3000. !cgs	
ch2o + oh	= hco + h2o	2.430e+10	1.20	-447. !cgs	09
ch2o + ho2	= hco + h2o2	3.000e+12	0.00	8000. !cgs	12
ch2o + m	= co + h2 + m	6.250e+15	0.00	69540. !cgs	
ch2o + m	= hco + h + m	4.000e+23	-1.66	91120. !cgs	
!h2 + co	= ch2o	4.300e+07	1.50	79600. !cgs	
hco + hco	= ch2o + co	3.010e+13	0.00	0. !cgs	
hco + oh	= h2o + co	1.000e+14	0.00	0. !cgs	
hco + h	= h2 + co	1.190e+13	0.30	0. !cgs	
hco + o	= oh + co	3.000e+13	0.00	0. !cgs	
hco + o	= h + co2	3.000e+13	0.00	0. !cgs	
hco + o2	= ho2 + co	3.300e+13	-0.40	0. !cgs	
hco + m	= h + co + m	1.870e+17	-1.00	17000. !cgs	
!hco + h + m	= ch2o + m	1.000e+12	0.48	-260. !cgs	
hco + ho2	= co2 + oh + h	3.000e+13	0.00	0. !cgs	
ch4 + o2	= ch3 + ho2	7.900e+13	0.00	56000. !cgs	
!ch3 + ho2	= ch4 + o2	1.000e+12	0.00	0. !cgs	
ch4 + h	= ch3 + h2	6.600e+08	1.60	10840. !cgs	
ch4 + oh	= ch3 + h2o	1.600e+06	2.10	2460. !cgs	
ch4 + o	= ch3 + oh	1.020e+09	1.50	8604. !cgs	99
ch4 + ho2	= ch3 + h2o2	1.000e+13	0.00	18700. !cgs	100
ch4 + ch2	= ch3 + ch3	4.000e+12	0.00	-570. !cgs	101
ch3 + ch2o	= ch4 + hco	5.500e+03	2.80	6000. !cgs	102
ch3 + hco	= ch4 + co	1.200e+14	0.00	0. !cgs	103
ch3 + h	= ch4	1.900e+36	-7.00	9050. !cgs	104
ch3 + h	= ch2 + h2	9.000e+13	0.00	15100. !cgs	105
ch3 + ch3o	= ch4 + ch2o	4.300e+14	0.00	0. !cgs	106 3.3
ch3 + ch3	= c2h6	2.700d+53	-12.0	19400. !cgs	
ch3 + ch3	= c2h5 + h	4.990e+12	.100	10600. !cgs	
!ch2 + h2	= ch3 + h	5.000e+05	2.00	7230. !cgs	
ch2 + oh	= ch2o + h	2.500e+13	0.00	0. !cgs	107

ch2 + o2	= hco + oh	4.300e+10	0.00	-500.	!cgs 108
ch2 + o2	= co2 + h2	6.900e+11	0.00	500.	!cgs 109
ch2 + o2	= co + h2o	2.000e+10	0.00	-1000.	!cgs 110
ch2 + o2	= ch2o + o	5.000e+13	0.00	9000.	!cgs 111
ch2 + o2	= co2 + h + h	1.600e+12	0.00	1000.	!cgs
ch2 + o2	= co + oh + h	8.600e+10	0.00	-500.	!
ch2 + ch2	= c2h2 + h2	1.200e+13	0.0	800.	!
ch2 + ch2	= c2h2 + h + h	1.200e+14	0.0	800.	!
ch2 + co2	= ch2o + co	1.000e+11	0.00	1000.	!cgs 112
ch3 + hco	= ch2o + ch2	3.000e+13	0.00	0.	!cgs 113
ch3 + c2h4	= ch4 + c2h3	6.620e+00	3.70	9482.	!cgs 114
ch3 + ch3	= c2h4 + h2	1.000e+15	0.00	31000.	!cgs 115
ch3 + ch2	= c2h4 + h	3.000e+13	0.00	-570.	!cgs 116
c2h4 + h	= c2h3 + h2	1.100e+14	0.00	8500.	!cgs 117
c2h4 + o	= ch3 + hco	1.600e+09	1.20	746.	!cgs 118
c2h4 + o	= ch2o + ch2	3.000e+04	1.88	180.	!cgs 119
c2h4 + o	= c2h3 + oh	1.510e+07	1.91	3790.	!cgs 120
c2h4 + oh	= ch2o + ch3	6.000e+13	0.0	960.	!cgs 121 ! 13
c2h4 + ho2	= c2h3 + h2o2	7.100e+11	0.0	17110.	!cgs 122
c2h4 + oh	= c2h3 + h2o	8.020e+13	0.00	5955.	!cgs 123 ! 6.02 5955
c2h4 + m	= c2h2 + h2 + m	1.500e+15	0.00	55800.	!cgs 124
c2h4 + m	= c2h3 + h + m	2.600e+17	0.0	96570.	!cgs 125
c2h4 + h	= c2h5	2.600e+43	-9.25	52580.	!cgs 126
c2h6 + o2	= c2h5 + ho2	1.000e+13	0.00	48960.	!cgs 127
c2h5 + o2	= c2h4 + ho2	2.000e+10	0.0	-2200.	!cgs 128
c2h4 + o2	= c2h3 + ho2	4.200e+14	0.00	57590.	!cgs 128 ! 14
c2h4 + c2h4	= c2h5 + c2h3	5.000e+14	0.0	64700.	!cgs 129 ! 14
c2h5 + ho2	= c2h4 + h2o2	3.000e+11	0.00	0.	!cgs 130
c2h2 + o2	= hco + hco	4.000e+12	0.00	28000.	!cgs 2.0
c2h2 + o	= ch2 + co	1.020e+07	2.00	1900.	!cgs 131
c2h2 + h + m	= c2h3 + m	5.540e+12	0.00	2410.	!cgs 132
c2h3 + h	= c2h2 + h2	4.000e+13	0.00	0.	!cgs 133
c2h3 + o2	= ch2o + hco	4.000e+12	0.00	-250.	!cgs 134
c2h3 + oh	= c2h2 + h2o	3.000e+13	0.00	0.	!cgs 135

c2h3 + ch2	= c2h2 + ch3	3.000e+13	0.00	0. !cgs	136
c2h3 + hco	= c2h4 + co	6.034e+13	0.0	0. !cgs	137
c2h3 + c2h3	= c2h2 + c2h4	1.450e+13	0.0	0.0	
c2h3 + o	= c2h2 + oh	1.000e+13	0.0	0.0	
c2h2 + oh	= ch3 + co	4.830e-04	4.00	-2000. !cgs	138
c2h3	= c2h2 + h	4.600e+40	-8.80	46200.	

end.

