



A numerical investigation of the effects of combustion parameters on the performance of a compression ignition engine toward NO_x emission reduction



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ABSTRACT

In this paper, a detailed multi-dimensional simulation based on fuel chemical reactions has been presented to investigate the effects of the most important parameters on performance and emission of a reactivity controlled compression ignition (RCCI) engine. The different characteristics of combustion phasing such as start of combustion, combustion duration, and 10%–90% of mass fraction burned (MFB) for iso-octane/n-heptane fuels have been studied. The effects of each important parameter such as amount of fuel delivered by varying fuels ratio, engine load and speed, injection timing, equivalence ratio, exhaust gas recirculation (EGR) application, boost pressure, injection pressure as well as combination of these different parameters and improved fuel octane number at higher compression ratios were evaluated to discover the most effective parameter on performance and emission of an RCCI engine. Distribution and coefficient of variation (COV) of equivalence ratio were examined in base cases to evaluate the influence of high reactivity fuel on distribution points. In addition, to acquiring a comprehensive perception, the results highlighted that by concurrently applying different parameters with diverse effects, new corridors to significantly abate nitrogen oxides (NO_x) pollutant can be achievable depending on the specific situations. Generally, the parameters that prolong the combustion duration demonstrated positive effects on combustion process leading to cleaner combustion with lower engine-out NO_x.

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1. Introduction

The possibility of controlling the fuel reactivity could be a very effective tool to control the combustion phases at different loads and speeds with no contradiction to have a homogenous and pre-mixed charge, consequently, significant and simultaneous reduction of NO_x and soot emissions is possible.

NO_x emission as one of the most prevalent engine-out pollutants is detrimental to good health and can lead to multifarious respiratory difficulties such as inflammation of the airways and aggravation of response to allergens. In addition to having destructive impacts on vegetation, NO_x can also react with other pollutants in the presence of sunlight to form harmful molecules of

ozone as well as acid rain, all threatening to human health in direct or indirect ways. Accordingly, evaluation of the ways to reduce NO_x emission is of great importance. Therefore finding new approaches of NO_x abatement has been widely paid attention in this study as well as previous researches.

Major research work is being carried out in RCCI engines due to significant potential in fuel consumption and emission reduction. Experimental or numerical parametric studies are a great part of these works as well as the efforts to examine new additives or surrogate fuels.

Numerous researches have been carried out in order to evaluate the effects of each parameter to effectively improve combustion phase in RCCI engines. Ma et al. (2013) evaluated the effects of multiple injection strategies on combustion phase in an RCCI engine in diverse operation conditions and reported high efficiency and low engine-out pollutants. The second injection in a double injection strategy was also introduced as a practical way to expand the engine operation limits to higher loads.

A parametric study carried out by Li et al. (2014) on the effects of

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Abbreviations

ATDC	After Top Dead Center
BTDC	Before Top Dead Center
CA	Crank Angle
CFD	Computational Fluid Dynamic
CNG	Compressed Natural Gas
CO	Carbon Monoxide
CO ₂	Carbon Dioxide
COV	Coefficient of Variation
EGR	Exhaust Gas Recirculation
EPA	Environmental Protection Agency

ER	Equivalence Ratio
HCCI	Homogeneous Charge Compression Ignition
IMEP	Indicated Mean Effective Pressure
MFB	Mass Fraction Burned
NO _x	Nitrogen Oxides
RCCI	Reactivity Controlled Compression Ignition
RPM	Revolutions Per Minute
SFC	Specific Fuel Consumption
SOI	Start of Injection
TDC	Top Dead Center
UHC	Unburned Hydrocarbon

1st and 2nd start of injection (SOI) timing and injection duration, diesel fuel mass fraction and natural gas mass fraction on a CNG/diesel RCCI engine. The second SOI timing and injection duration were found out to be the most crucial factors which can well improve indicated power output. Using adaptive injection strategies, [Hanson et al. \(2016\)](#) studied parameters such as main and pilot SOI timing, EGR rate, port fuel injection mass fraction and rail pressure to extend the RCCI engine operation limit to higher loads. Also, they realized that conventional diesel combustion and RCCI combustion have same sensitivities toward direct injection parameters. Except for NO_x, almost all emissions were seen to be benefited from using no EGR. Besides, thermal efficiency was slightly improved.

[Walker et al. \(2012\)](#) fueled an RCCI engine with a low pressure gasoline direct injection fueling system which is economically justifiable and compared the results with a high pressure (common rail injection) system. The results were observed to be comparable in emissions except for unburned hydrocarbons (UHC) due to hampered mixture formation and combustion efficiency. In another experimental work, [Benajes et al. \(2015\)](#) found the diesel fuel injection timing, EGR rate and fuel blending ratio as the key variables to reach to stable RCCI engine operation. They observed great dependency of NO_x and soot to engine speed and diesel fuel SOI, respectively. It was claimed that lowering the compression ratio from 14.4:1 to 11:1 can result in great improvements in UHC, carbon monoxide (CO) and soot emissions.

By developing a 3D-CFD combustion model, [Nazemi and Shahbakhti \(2016\)](#) optimized the effects of four different parameters including: spray angle, SOI timing, injection pressure and pressure rise rate on combustion and performance of an RCCI engine and found out that spray angle and injection pressure have the most and the least effects on RCCI combustion and performance.

[Kalsi and Subramanian \(2016\)](#) carried out experimental tests on a diesel/CNG RCCI engine with different levels of EGR and demonstrated a noticeable reduction in CO and UHC emissions (which are problematic at part load in RCCI engines) as well as further NO_x reduction while a level of 8% EGR was implemented, although soot emission was seen to get slightly increased.

[Kakae et al. \(2015\)](#) modeled a heavy duty CNG/diesel RCCI combustion engine to investigate the effects of fuel composition, engine speed and initial temperature on performance and emission. They found out that the higher energy flow rate of low reactivity fuel through a fixed orifice results in higher peak pressure, temperature and NO_x emission but still the gas with higher energy flow rate was mentioned to be more favorable at higher engine speeds to avoid incomplete combustion.

The surrogate fuels have been immensely subjected to RCCI engines studies. They are of disparate octane and cetane numbers as well as diverse reactivity levels; among the common surrogate

fuels used for RCCI engines, ethanol and hydrous ethanol fuels were investigated in ([Curran et al., 2014](#); [Splitter et al., 2011b](#)). [Splitter et al. \(2011a\)](#) replaced gasoline fuel by E85 in a gasoline/diesel fueled RCCI engine and reported a 12% increase in indicated mean effective pressure (IMEP) and a 3% improvement in thermal efficiency due to less EGR demand. As well as expanding the engine load operation range, [Curran et al. \(2012\)](#) elucidated that employing ethanol fuel in the RCCI engine results in further retard in the start of low-temperature reactions and consequently in combustion phase. The UHC pollutant was seen to get reduced by injecting more amount of diesel fuel. [Dempsey et al. \(2012\)](#) investigated the effects of different levels of hydrous ethanol fuel in an RCCI engine and pointed out that as well as reduction in in-cylinder primary temperature, the presence of water in the fuel can also lead to the enhancement of engine gross thermal efficiency up to 55%. The combination of 70% ethanol fuel and 30% water (by mass) was also found to have the capability of significantly changing the engine operation limits without using EGR. [Qian et al. \(2015\)](#) experimentally investigated the specifications of gasoline/diesel and ethanol/diesel RCCI engines and demonstrated that employing ethanol fuel instead of gasoline fuel as port injected fuel can remarkably reduce NO_x emission due to high latent heat of the fuel and resulted in longer ignition delay. Also replacing gasoline fuel by an oxygenated fuel can immensely mitigate the particulate matter production although UHC pollutant gets increased. [Tong et al. \(2016\)](#) conducted experimental investigations on a polyoxymethylene dimethyl ethers/gasoline RCCI engine and compared its characteristics to a diesel/gasoline one. It was pointed out that significant improvements in IMEP and indicated thermal efficiency, as well as soot reduction can be achieved by using polyoxymethylene dimethyl ethers as the directly injected high reactivity fuel with slightly higher but still comparable NO_x emission. [Lu et al. \(2013\)](#) proposed a two-stage sequential combustion mode using n-heptane as diesel-type fuel and four fuels (i.e., iso-octane, ethanol, iso-propanol, 1-butanol) as gasoline-type fuels and compared and contrasted the effects of different gasoline-type fuels on heat release and emission reduction. They reported the similar level of produced NO_x in all four cases while the engine fueled with n-heptane/iso-octane fuels was found to produce the most amount of soot. An experimental investigation on performance and emissions of a high speed diesel engine fueled with n-butanol/diesel blends was carried out by [Valentino et al. \(2012\)](#). It was concluded n-butanol-diesel fuels (20% and 40% of n-butanol by volume) blends that are highly volatile and highly resistant to spontaneous ignition, can improve engine emissions with not much penalties in specific fuel consumption or mean effective pressure.

[Zhou et al. \(2015a\)](#) numerically investigated the knock tendency of a methanol/biodiesel RCCI engine. High levels of cooled EGR, retarded SOI and fewer fractions of methanol fuel were found to

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