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A numerical investigation of the effects of combustion parameters on the performance of a compression ignition engine toward NOx 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.

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 premixed 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.

Kakaee 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-butanul/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 minimize the knocking intensity. It was also concluded that HCO and OH radicals are important intermediate species in the occurrence of knocking. In another work, Zhou et al. (2015b) simulated the combustion phase of a methanol/biodiesel RCCI engine by a 3D-CFD model and investigated the effects of variations in the amount of ethanol fuel mass fraction at different loads. By increasing methanol fuel at under 10% load conditions, they showed a decrease in the peak pressure and heat release rate as well as a slight increase in CO and a significant drop in NO_x production while 60% methanol fuel induction resulted in peak pressure at both loads under 50% and 100%. Park and Yoon (2016) experimentally used diesel-gasoline and diesel-biogas dual fuel combustion strategies for a compression ignition engine and kept the combustion mode quite similar to RCCI engines. They observed that the increase in port injection ratio and its rate can enhance the IMEP even close to the operation of a conventional diesel. Besides, it prolonged the combustion delay which was more obvious in diesel-biogas case.

Based on the literature, some parameters such as the location of the start of combustion and combustion duration with regard to its efficiency and other combustion characteristics in an RCCI engine still need to be looked more closely. Besides, the better understanding of the RCCI concept requires a general look toward all substantial parameters applied concurrently, as well as a multilateral compare and contrast of the effects of each parameter in order to find the best configurations of them to maximize the produced power as well as mitigating the NO_x emission.

Therefore this study aims to focus on more than 10 influential parameters and investigates their effects on the start of combustion, combustion duration, and NO_x production to deepen our perception from combustion process by implementing a 3D model and CFD analysis on a heavy duty RCCI engine fueled with iso-octane and n-heptane fuels. In continuation, ethanol fuel was employed as a surrogate fuel to present more diverse approaches to reducing emissions and to demonstrate a more palpable depiction of combustion process in such engines.

2. Numerical model and validation

In this work, The CONVERGE CFD tool (Richards et al., 2014) was used for closed-loop simulation of a single cylinder Cat® 3401E SCOTE RCCI engine. Further specifications of the engine are listed in Table 1. The injector nozzle is of 6 holes for better mixing effect. Thus, a 60° sector of the combustion chamber shown in Fig. 1 was used as a compromise between accuracy and computational runtime. A reduced chemical reaction mechanism of 113 species and 487 reactions was used for combustion model (Ra and Reitz, 2011). Based on previous studies, it is quite reasonable to use iso-octane fuel as gasoline-type fuel and n-heptane fuel as diesel fuel (Ra et al., 2009). The port injected iso-octane fuel is considered to be homogeneously mixed and vaporized at intake valve close and n-heptane fuel is injected directly into the cylinder which is simulated by numerous models. The No Time Counter method was used to simulate collision process (Schmidt and Rutland, 2000). The spray coalescence was simulated using the O'Rourke collision model (O'Rourke, 1981). For wall impingement simulation, the model developed by Naber and Reitz (1988) and also Gonzalez et al. (1992) was used which includes two impingement regimes based on the Weber number. The hybrid Kelvin-Helmholtz Rayleigh-Taylor model was also applied to simulate spray atomization and break-up processes (Reitz and Bracco, 1986; Reitz, 1987). In order to include detailed chemistry in combustion applications, the SAGE model (Senecal et al., 2003) was added. Soot was predicted using a phenomenological soot model based on the Hiroyasu research (Hiroyasu and Kadota, 1976). NO_x emission were estimated by means of a reduced NO mechanism (Sun, 2007), developed based on the GAS Research Institute (GRI) NO mechanism method (Smith et al., 1999).

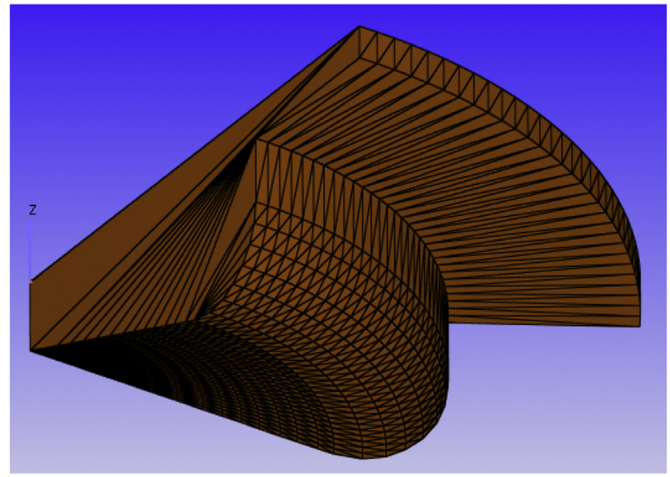

Fig. 1. A 60° sector of engine cylinder geometry.

To validate the abovementioned 3D model, the experimental data was taken from a similar work which was carried out at the Engine Research Center (University of Wisconsin-Madison). The engine has been equipped with two injectors, one for port injection of low reactive fuel (i.e. gasoline fuel) and one for in-cylinder direct injection of high reactive fuel (i.e. diesel fuel). The fuel injection system specification is presented in Table 2.

The experimental test conditions and experimental results are tabulated in Tables 3 and 4, respectively.

The in-cylinder pressure and heat release rate comparison of the developed model and the experiments are depicted in Figs. 2–4. The simulation results are in good agreement with the experimental results both in trends and values.

The predicted emissions of the model and experimental data are depicted in Fig. 5, again there is a reasonable agreement both in trends and values.

3. Results and discussions

3.1. The selected primary cases

The different parameters affecting the start of combustion and

Table 1
Specification of Wisconsin – Madison ERC diesel engine (Splitter, 2010).

Cat® 3401E SCOTE engine geometry	
Cylinder Volume (Liter)	2.44
Cylinder Bore (cm)	13.72
Connecting Rod Length (cm)	21.16
Geometrical Compression Ratio	16.1
Number of Valves in Cylinder	4
Intake Valve Closing (°ATDC)	−143 and −85
Exhaust Valve Opening (°ATDC)	130

Table 2
Specification of low and high pressure injectors (Splitter, 2010).

Low pressure injector	
Injection Pressure (bar)	5.17
High pressure Injector	
Number of Nozzle at Injector	6
Nozzle Bore (μm)	250
Injector Pressure (bar)	800

Table 3
Engine test conditions (Kokjohn et al., 2011; Splitter, 2010).

Engine characteristics	Specification		
	Case1	Case2	Case3
Engine Speed (RPM)	1300	1300	1300
EGR Rate (%)	0	0	46
Equivalence Ratio	0.33	0.24	0.78
Intake Air Temperature (°C)	32	32	32
Intake Air Pressure (bar)	1.03	1.37	2
Total Fuel (mg)	53	60.1	125
Percent Gasoline by Mass (mg)	48%	68%	85%
Diesel Injection Pressure (bar)	400	800	800
Start of Diesel Injection in Pulse1 (°ATDC)	−62	−58	−67
First Injection Duration (°CA)	9.4	5.04	5.1
Amount of Diesel Fuel in Pulse1	65%	68%	68%
Start of Diesel Injection in Pulse2 (°ATDC)	−37	−37	−36
Second Injection Duration (°CA)	5.1	2.34	2.3
Intake Valve Closing (°ATDC)	−85	−143	−85

Table 4
Experimental results (Kokjohn et al., 2011; Splitter, 2010).

Engine characteristics	Case1	Case2	Case3
GI[a] Power (kW)	12.15	13.63	30.6
GI SFC (gr/kW-h)	170	172	159
GI MEP (bar)	4.6	5.16	11.6
GI Nitrogen Oxide (gr/kW-h)	0.024	0.01547	0.0094
GI Soot (gr/kW-h)	0.001	0.00516	0.0076

[a] Gross Indicated.

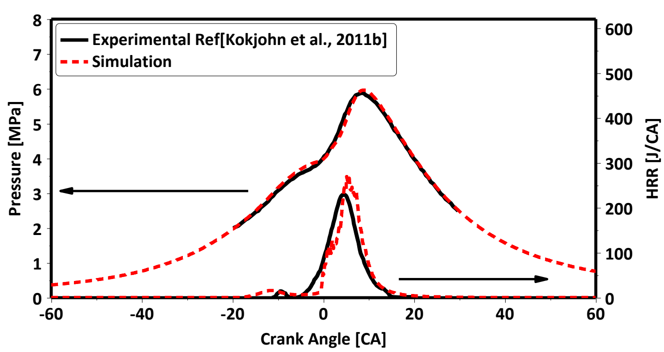

Fig. 2. Comparison between simulation and experimental results for in-cylinder pressure and heat release rate in the case 1.

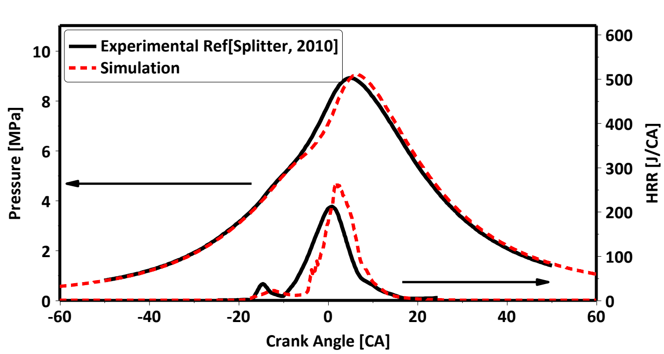

Fig. 3. Comparison between simulation and experimental results for in-cylinder pressure and heat release rate in the case 2.

combustion duration in RCCI engines fueled with iso-octane and n-heptane fuels were investigated. In this study, it is intended to look at all the major effective parameters and find a practical procedure

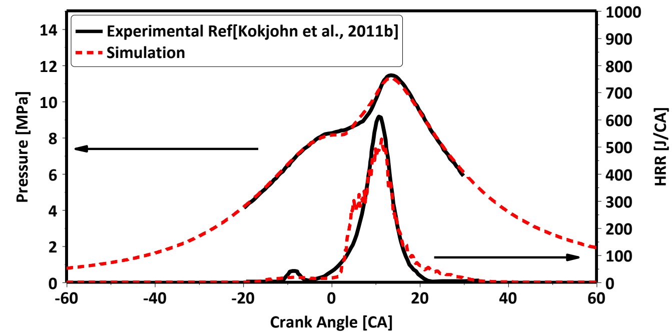

Fig. 4. Comparison between simulation and experimental results for in-cylinder pressure and heat release rate in the case 3.

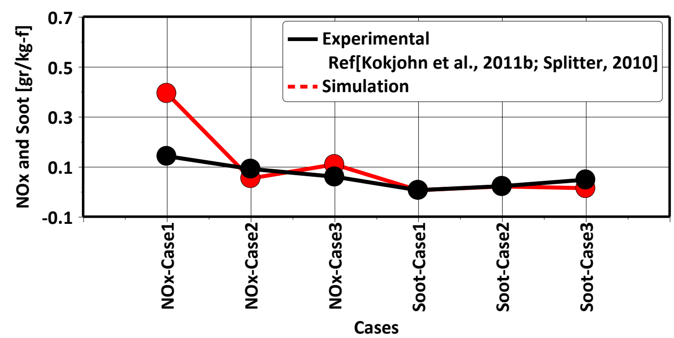

Fig. 5. Comparison between simulation and experimental results for in-cylinder emissions in the cases 1 to 3.

to improve the performance of the RCCI engine and to achieve a global view of the start of combustion and combustion duration to exert a multilateral control strategy. Other combustion specifications such as engine emission levels, the start and duration of n-heptane and iso-octane fuels consumption and combustion efficiency also were investigated.

To achieve this goal nine different primary cases of engine performance points have been chosen (Table 5). In these cases, increasing the amount of total fuel, varying in fuels ratio, changing engine speed, and injection timing are considered. Other different

Table 5
9 Different primary cases for investigating the effects of different parameters.

Cases	Fuel		Speed [RPM]	Injection Timing [bTDC]		Lambda
Case A	Total [mg]	70	1300	Pulse1	58	0.294
	Iso-octane [%]	68		Pulse2	37	
Case B	Total [mg]	70	1300	Pulse1	58	0.294
	Iso-octane [%]	82		Pulse2	37	
Case C	Total [mg]	100	1300	Pulse1	58	0.42
	Iso-octane [%]	68		Pulse2	37	
Case D	Total [mg]	100	1300	Pulse1	58	0.42
	Iso-octane [%]	82		Pulse2	37	
Case E	Total [mg]	100	1700	Pulse1	58	0.42
	Iso-octane [%]	68		Pulse2	37	
Case F	Total [mg]	100	2100	Pulse1	58	0.42
	Iso-octane [%]	68		Pulse2	37	
Case G	Total [mg]	100	1300	Pulse1	48	0.42
	Iso-octane [%]	68		Pulse2	27	
Case H	Total [mg]	100	1300	Pulse1	38	0.42
	Iso-octane [%]	68		Pulse2	17	
Case I	Total [mg]	100	1300	Pulse1	68	0.42
	Iso-octane [%]	68		Pulse2	47	

Table 6
Different investigated parameters for applying on 9 primary cases.

No.	Investigated Parameter	Quantity
1	Increased in Equivalence Ratio	10%
2	Increased in Equivalence Ratio	20%
3	Decreased in Equivalence Ratio	15%
4	Decreased in Equivalence Ratio	30%
5	EGR Without Boost Pressure	20%
6	EGR Without Boost Pressure	40%
7	EGR With Boost Pressure	20%
8	EGR With Boost Pressure	40%
9	Increased in Injection Pressure	1100 bar
10	Increased in Injection Pressure	1400 bar
11	Replacing Iso-octane by Ethanol fuel and increasing CR	20% and 17.5
12	EGR Without Boost Pressure and increasing CR	40% and 17.5

parameters were applied to these nine primary cases in order to investigate the engine combustion characteristics in details (Table 6).

As shown in Table 5, the mass ratio of iso-octane fuel to total fuel in case B has been increased in proportion to case A. In cases C and D, the ratio of two fuels is the same as cases A and B respectively, but the total mass has been increased to 30 mg. In other cases, all changes have been made with respect to case C. The speed has been increased in cases E and F and in next three cases, the injection timing has been changed.

For ease of comparison, the combustion characteristics of primary cases are depicted in Fig. 6. The amount of peak pressure got decreased and the point of maximum in-cylinder pressure was retarded in cases B and D in comparison to cases A and C due to increasing in iso-octane/n-heptane fuels ratio.

In cases E and F, the speed has been increased while the n-heptane fuel injection timing stayed constant, it can be seen that in these cases, the combustion duration has been protracted and consequently, the amount of peak pressure has been reduced and the occurrence of peak pressure has been retarded. In the last three cases where the injection timing is changed while the total fuel mass and iso-octane to n-heptane fuels ratio are kept constant, it is seen that the peak pressure in cases G and H are slightly higher than case C, however, its occurrence has been advanced. The reason is the fact that by retarding the injection of high reactive fuel, there would be less time available for the mixture to get homogenous so the number of regions with relative high reactivity, increases. Hence the ignition occurs earlier, so in these cases, the peak pressure point occurs near TDC. This also means that any injection retardation in an RCCI engine should be made wisely since cases G and H deal with a high average temperature and extended ringing intensity. This is why these cases are among 9 cases that get sensible improvement by other parameters and these important circumstances are explained in details as follows.

In RCCI engines, the low reactive fuel is injected into the intake port and gets perfectly premixed during intake and compression strokes so it can be assumed that before the start of high reactive fuel injection, the equivalence ratio is uniform in all regions within the combustion chamber. Immediately after the injection of the second fuel, the equivalence ratio (of two fuels) within the chamber forms a gradient from regions containing the high amount of secondary fuel to regions which are devoid of it. The occurrence of ignition and continuation of combustion in RCCI engines is based on this gradient of equivalence ratio so that starts from rich zones of high reactive fuel and stretches to lean zones. The more time provided for the high reactive injected fuel before the start of combustion to form a homogenous mixture, the less gradient of equivalence ratio is formed and vice versa. The best way to demonstrate the gradient of equivalence ratio is using "standard deviation of equivalence ratio" within the cylinder.

More aggregation of high reactive zones within the combustion chamber results in more deviation of maximum equivalence ratio from the average value. While combustion delay is prolonged and therefore, the secondary fuel gets more premixed, the amount of

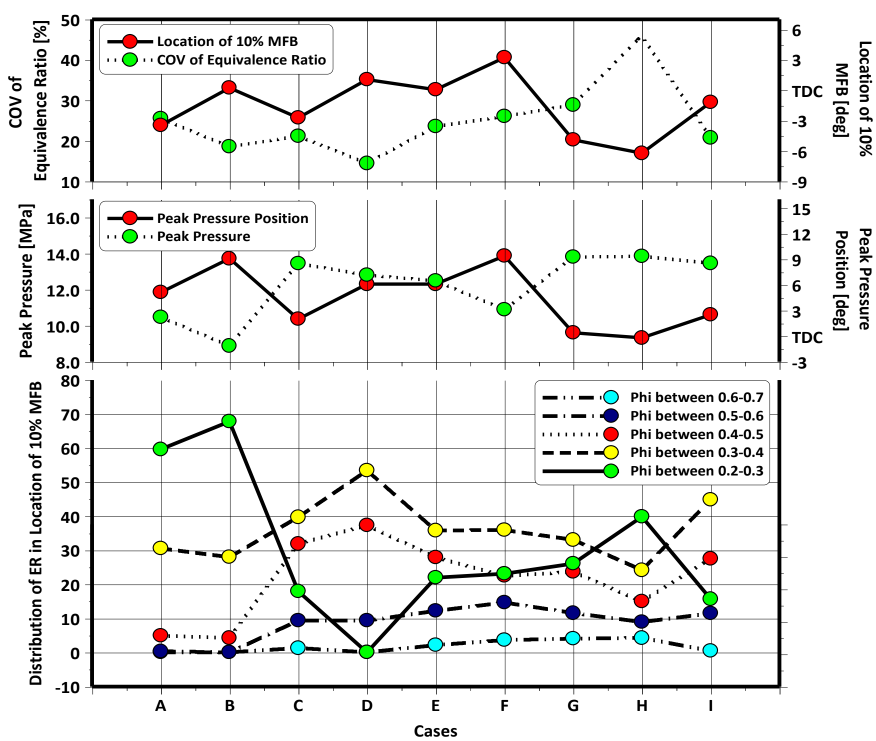

Fig. 6. The location of 10% MFB, COV of equivalence ratio, peak pressure position, peak pressure and distribution of ER in the location of 10% MFB in the base cases.

this deviation reduces. The standard deviation of equivalence ratio can be calculated by the following relations.

$$\varnothing_{STD} = \sqrt{\frac{\sum_{cell} m_{cell}(\varnothing_{cell} - \varnothing_{mean})^2}{m_{total}}} \tag{1}$$

$$\varnothing_{cell} = \frac{2\sum_i N_i \eta_{C,i} + \frac{1}{2}\sum_i N_i \eta_{H,i}}{\sum_i N_i \eta_{O,i}} \tag{2}$$

$$\varnothing_{mean} = \frac{\sum_j 2\sum_i N_i \eta_{C,i} + \frac{1}{2}\sum_i N_i \eta_{H,i}}{\sum_j \sum_i N_i \eta_{O,i}} \tag{3}$$

In order to assign a specific number for the relation of standard deviation, COV of the equivalence ratio is used which can be obtained via the following relation.

$$COV = (\varnothing_{STD}/\varnothing_{mean}) \times 100 \tag{4}$$

A high value for COV in a specific angle indicates that the high reactive fuel is accumulated within a few regions in the combustion chamber, so the probability of an advance in combustion phasing increases. Conversely, the less value for COV, the more retardation in combustion unless some other parameters such as increased in-cylinder temperature play a role like in the second case and make an advance in combustion.

The value of COV (used to indicate the mixture reactivity) has been calculated by the time that 10% heat is released. Fig. 6 shows the COV values for different cases. Relative to case A, the COV value for case B is lower since a fewer amount of n-heptane fuel has been injected. Hence a higher temperature is needed to initiate the combustion and this is why the combustion phase is retarded in case B. In a similar way, ignition delay in case D is longer than case C.

Relative to case C, there is a shorter time available for spray breakup and evaporation to form a homogenous mixture in cases E and F, so the COV values in these cases are definitely higher than that of case C. but on the other hand, with regard to increasing in engine speed, the start of heat release in cases E and F is retarded.

In cases G and H, the secondary fuel injection is retarded in comparison to case C. Therefore, the fuel droplets have not adequate time available to get totally mixed with the air-primary fuel mixture and surely in near TDC angles in cases G and H, the COV has a high value. Consequently, as can be seen in Fig. 6, the combustion is advanced in these cases.

In the last case, since the n-heptane fuel was injected earlier than in case C, a more homogeneous mixture has been formed and a lower value for COV has been obtained and as expected, the location of 10% mass fraction burned in case I has been retarded in comparison to case C.

The last part in Fig. 6 demonstrates the distribution of equivalence ratio in the location of 10% MFB. As can be seen, the equivalence ratio of primary fuel in cases C, E and after, is between 0.2 and 0.3 and as the injection gets nearer to TDC in cases G and H, the percentage of equivalence ratio increases to take an amount between of 0.6–0.7.

Our major attention in this research has been paid to the time of initiation of iso-octane and n-heptane fuels decomposition and the duration of these reactions as well as the start and duration of heat release. By investigating different parameters in this paper, a great effort was made to determine the effects of these parameters. Accordingly, the 9 primary cases were discussed in the following part.

As can be deduced from the chemical reactions kinetics, at first the bounds between C and H atoms are broken up via decomposition reactions and then the reactions of energy releasing take place. This is why an interval from 10% to 90% of iso-octane and n-heptane fuels decomposition is considered in all cases.

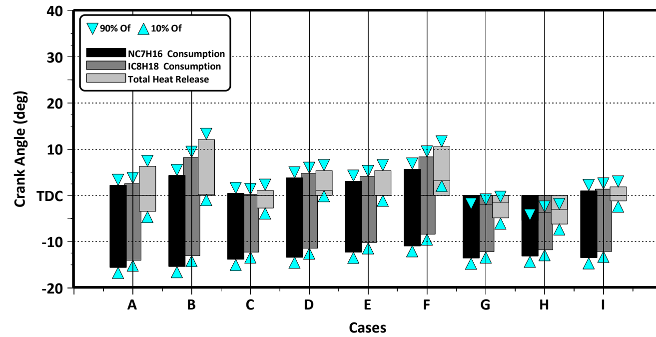

Fig. 7. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the base cases.

In Fig. 7, the consumption timing of n-heptane and iso-octane fuels is demonstrated as well as the timing of energy release. In most cases, n-heptane fuel starts to get consumed earlier than iso-octane fuel and also gets finished earlier since this is n-heptane fuel as high reactive fuel which forms the ignition within the mixture. The exception is cases A and C in which a higher quantity of n-heptane fuel is used and requires more time to get fully consumed.

In order to consider the cases more closely, the complete route of n-heptane and iso-octane fuels consumption is depicted in Fig. 8. According to Figs. 7 and 8 some important facts can be concluded as follows:

1 By Comparing cases C and D, it can be found that more than 60%–70% of n-heptane fuel in both cases has been burnt simultaneously because of the in-cylinder temperature increases due to volume shrinkage in the compression stroke. The significant difference about n-heptane fuel consumption between cases C and D are related to the last 30%–40% of n-heptane fuel mass. In case C, the combustion phase is advanced due to the higher amount of n-heptane fuel which creates zones with higher reactivity within the combustion chamber. An earlier heat release accelerates n-heptane fuel consumption and therefore the rest of the fuel is burnt in a shorter duration. However, a lower amount of n-heptane fuel is used in case D and that causes a longer delay in heat release which is why the rest of the fuel is burnt in a lower speed. One important point from Fig. 8 is the fact that about 20%–30% of iso-octane fuel is consumed before the main heat release, during low-temperature reactions as there is a slight heat release but with a relatively long delay, the rest of the fuel is burnt as the release of major energy which creates the main phase of combustion in RCCI engines. The process of iso-octane fuel consumption and heat release in cases A and B is also quite similar to cases C and D.
2 The heat release phase has been advanced in cases G and H since the injection of n-heptane fuel has been retarded which leads to the creation of regions with higher reactivity. This accelerates the consumption of both n-heptane and iso-octane fuels.
3 The consumption of both low and high reactive fuels has been retarded in cases E and F which is obvious in Figs. 7 and 8.

3.2. Investigation of the effects of changes in different parameters on engine performance

In the following sections, the start of combustion timing and

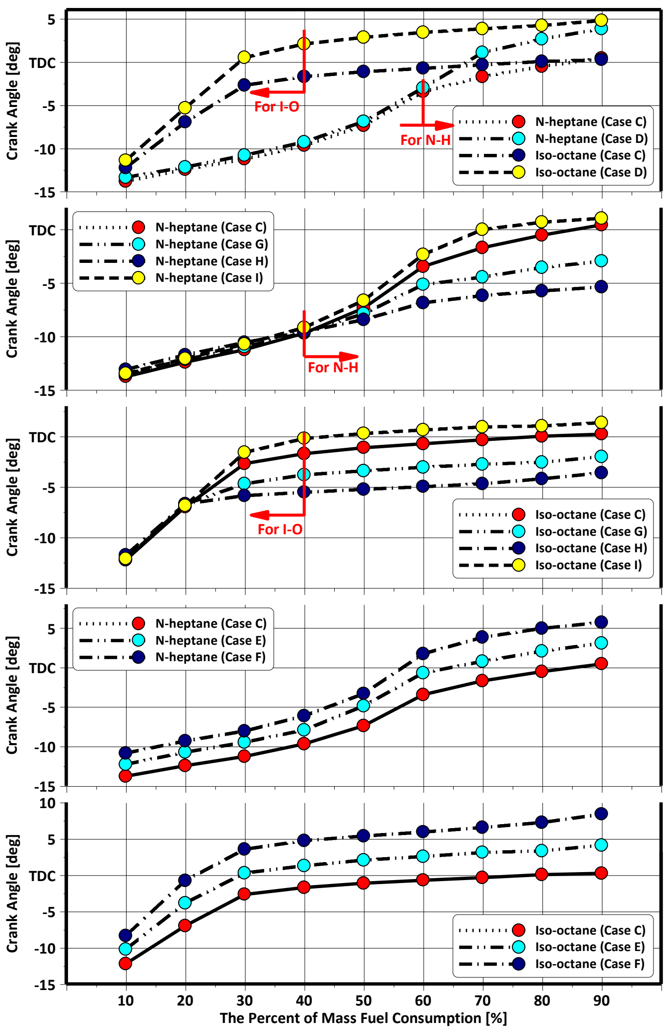

Fig. 8. The percent of mass fuel consumption from 10% to 90% in the base cases.

combustion duration for primary cases are investigated under different engine conditions as mentioned in Table 6 to find out the effect of influential parameters. All these parameters are considered in 9 primary cases, so the effects of each parameter on all these cases could easily be examined.

3.2.1. *The effects of equivalence ratio*

The amount of equivalence ratio (∅) was changed in two stages by altering the intake pressure in all cases in order to investigate its effect on each case. Initially, the equivalence ratio was equal to 0.294 for cases A and B and 0.42 for other cases. Then it was increased by 10% and 20% and reached to 0.325 and 0.465 after 10% increase and 0.355 and 0.599 after 20% increase in equivalence ratio, respectively. Next, by means of increasing boost pressure, the equivalence ratio was reduced by 15% (to became 0.25 for case A and B and 0.36 for other cases) and by 30% (to became 0.2 and 0.295, respectively).

The combustion results for iso-octane and n-heptane fuels and relevant heat releases are depicted in Figs. 9 and 10. Since the equivalence ratio has been changed through changing the intake air, another important parameter can be the spray penetration length due to changes in in-cylinder pressure and oxygen concentration and their effects on fuel jet breakup and evaporation process.

Finally, the mixing processes get accelerated so the spray penetration length is shortened and causes increase in number of high reactive zones where the first ignition cores could be created. The results for spray penetration length are shown in Fig. 11. Also enhancing the boost pressure reduces the in-cylinder temperature and increases the air density. This can firstly ignite the mixture with less delay and secondly convert the double-stage auto-ignition to a single-stage (Wissink and Reitz, 2015). In other words, while the start time of low-temperature reactions is constant (which is not affected by increasing boost pressure) and the time of high-temperature reactions is advanced, the time distance between low and high-temperature reactions vanishes. Also, in this situation, the importance of fuel cetane number in combustion gets diminished.

A high equivalence ratio increases the amounts of heat released in low-temperature reactions. This can be proved by the increase in the concentration of species such as H_2O_2, HCHO, and CO which are referred to as middling products.

Although the timing of both low and high-temperature reactions are advanced while the equivalence ratio is decreased, the combustion duration can be seen to get prolonged.

Fig. 9 exhibits the effects of increasing equivalence ratio in (two steps) on consumption duration of both low and high reactive fuels and also on heat release duration. As above mentioned, the decomposition process of both types of fuels and therefore the combustion phase has been retarded in all cases. As expected, in most cases, the combustion duration has become shortened; the exception is for cases F and B where the extreme ignition delay has retarded the combustion process to the expansion stroke. Hence, the combustion kinetics get modulated and the combustion duration gets excessively prolonged.

Increasing the equivalence ratio in cases C, G and H which consist higher reactive zones before combustion can be a notable choice to improve the engine performance since it can retard the combustion phase and help the heat to get released almost after TDC.

Fig. 10 refers to the results of reduction in amounts of equivalence ratio. As it was expected the combustion phase has been advanced and the combustion duration has been prolonged. The increase in air mass within the cylinder is seen to have an unfavorable effect on cases with the fewer mass of total fuel introduced into the combustion chamber (cases A and B), since part of fuel stays unburnt as a penalty in combustion efficiency. This fact is also evident in heat release diagram of cases A and B.

From the combustion duration point of view, both increasing and decreasing the equivalence ratio can improve the performance in cases D and G by significantly decreasing pressure rise rate and therefore reducing the ringing intensity in RCCI engines.

In Addition to considering the combustion duration which affects the engine noise and performance, NO_x emission is of importance and has been studied in all cases. Any changes in combustion duration and also in time of heat release initiation can notably affect the in-cylinder temperature. Fig. 12 illustrates the amounts of produced NO_x with respect to changes in values of equivalence ratio. The NO_x production in most cases has been escalated by increasing the equivalence ratio. On the contrary, reduction in equivalence ratio leads to less NO_x emission in most cases due to a drastic decline in temperature within the cylinder so that, in some cases such as A to E, the amounts of NO_x have reached to Environmental Protection Agency (EPA) 2010 standard and even lower levels.

3.2.2. *The effects of EGR*

The EGR effects wEre studied in two cases. Initially, EGR was increased by 20% and 40% of the primary cases and mixed with

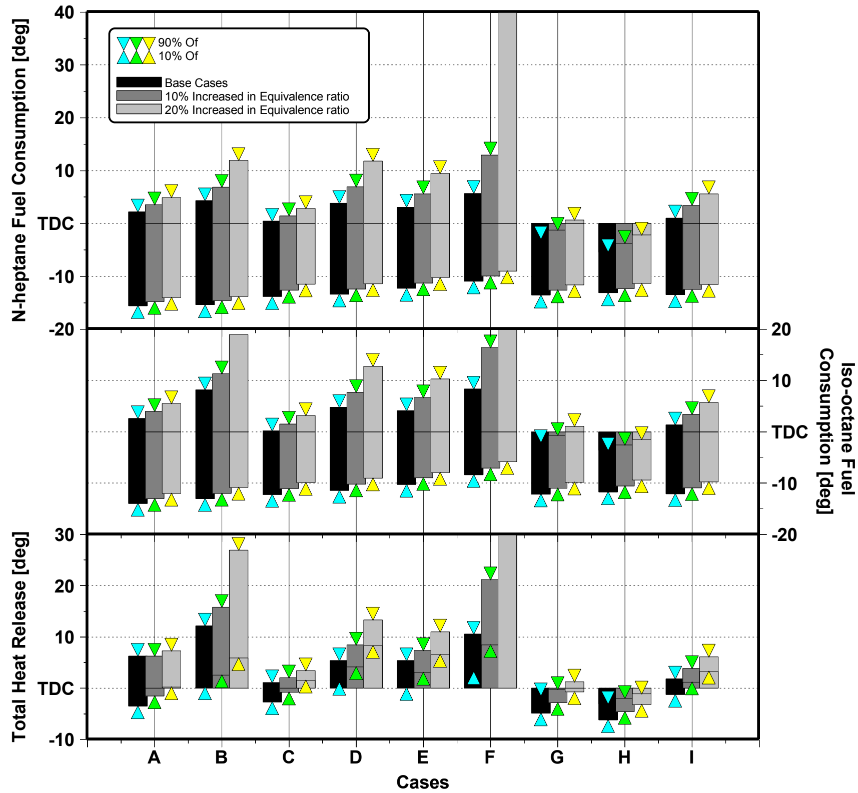

Fig. 9. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the cases with increasing equivalence ratio.

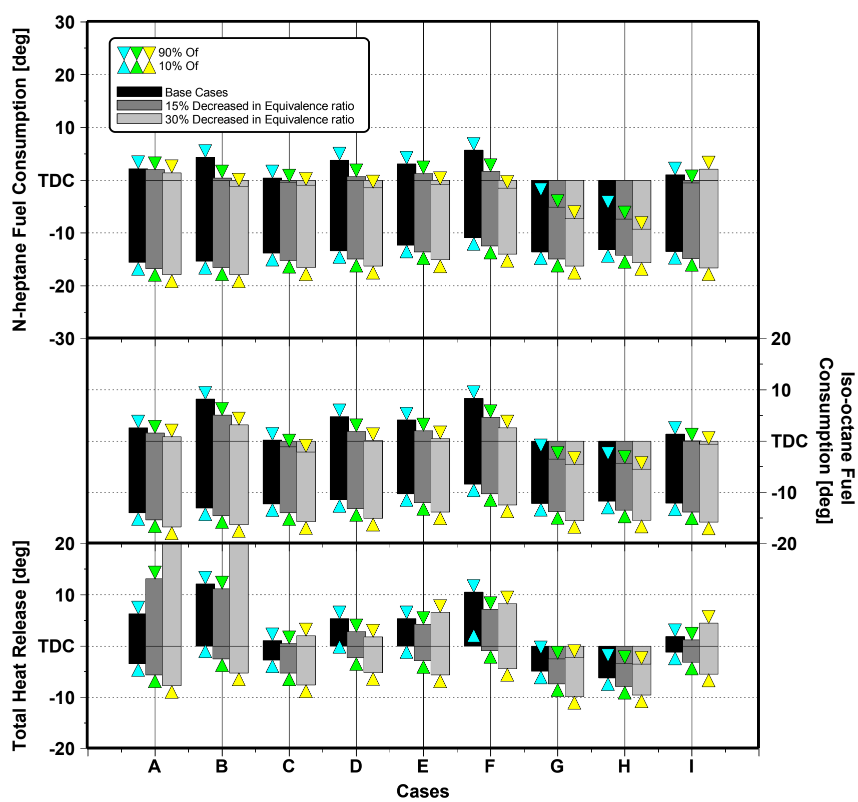

Fig. 10. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the cases with decreasing equivalence ratio.

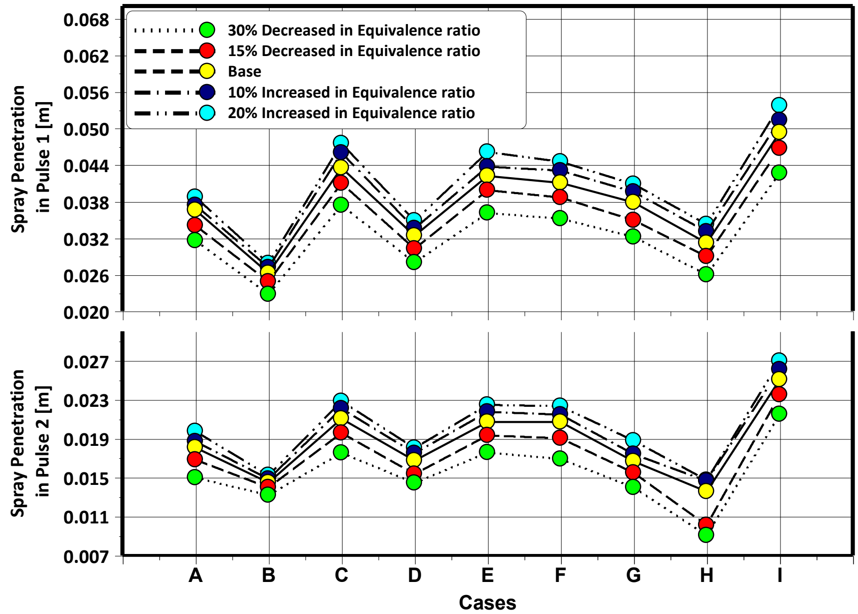

Fig. 11. Spray penetration in pulse 1 and 2 with increasing and decreasing equivalence ratio.

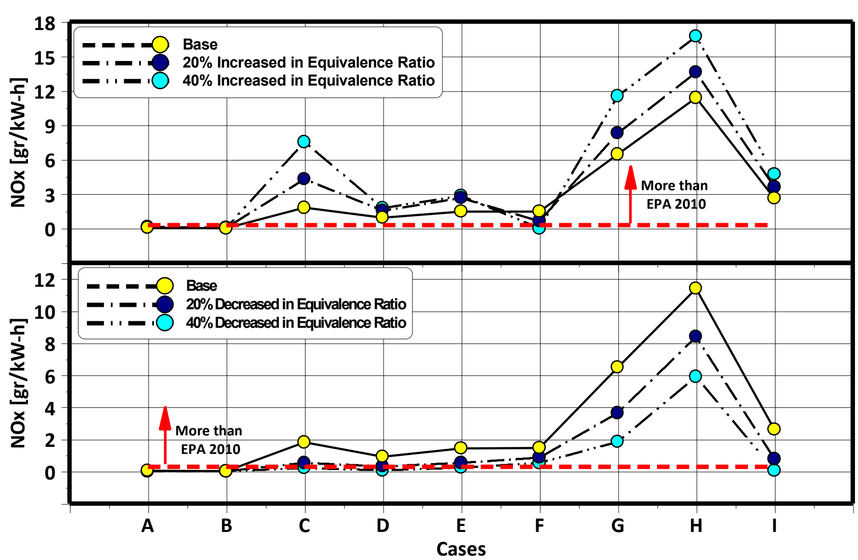

Fig. 12. NO_x production in the cases with increasing and decreasing equivalence ratio.

intake air with no boost pressure. In the other cases, the boost pressure was introduced to compensate the lack of intake air as a result of adding EGR. Cold EGR is used to neglect the heat exchange effects with the same temperature as intake air.

The results for n-heptane and iso-octane fuels consumption and total heat release in the case of 20% and 40% increase in EGR without boost pressure are shown in Fig. 13. This state is similar to the state of increasing equivalence ratio while the mass of intake air in both is relatively reduced. From oxygen concentration reduction point of view, the state of 10% increase in equivalence ratio is approximately comparable to the state of 20% increase in EGR level. Intake air concentration is reduced by 9.5% and 17.5% in the first and second stage, respectively, in the state of increasing equivalence ratio while it is reduced by 10% and 23% in two stages of enhancing EGR level. As shown in Fig. 13, a 20% EGR level has significant effects on performance of RCCI engine and extends combustion duration and combustion delay in cases C, G, and H in which the heat release is near TDC so a better combustion with less NO_x is achieved. However, by increasing the EGR level to 40%, it is evident in Fig. 13 that incomplete combustion occurs in most cases and the combustion efficiency is detracted.

The amounts of engine indicated efficiency are shown in Fig. 14 where a significant loss in combustion efficiency for cases D, E and F can be found while a 40% increase in EGR rate is implemented to the engine so that further increase in EGR rate is considered unfavorable.

With EGR, the concentration of species such as CO_2 and H_2O which exist in exhaust gasses increases within the cylinder. These gasses have higher heating values and can absorb more heat from the combustion chamber.

In the next stage, the effects of increasing EGR with the proportionate increase in boost pressure were investigated. Since the

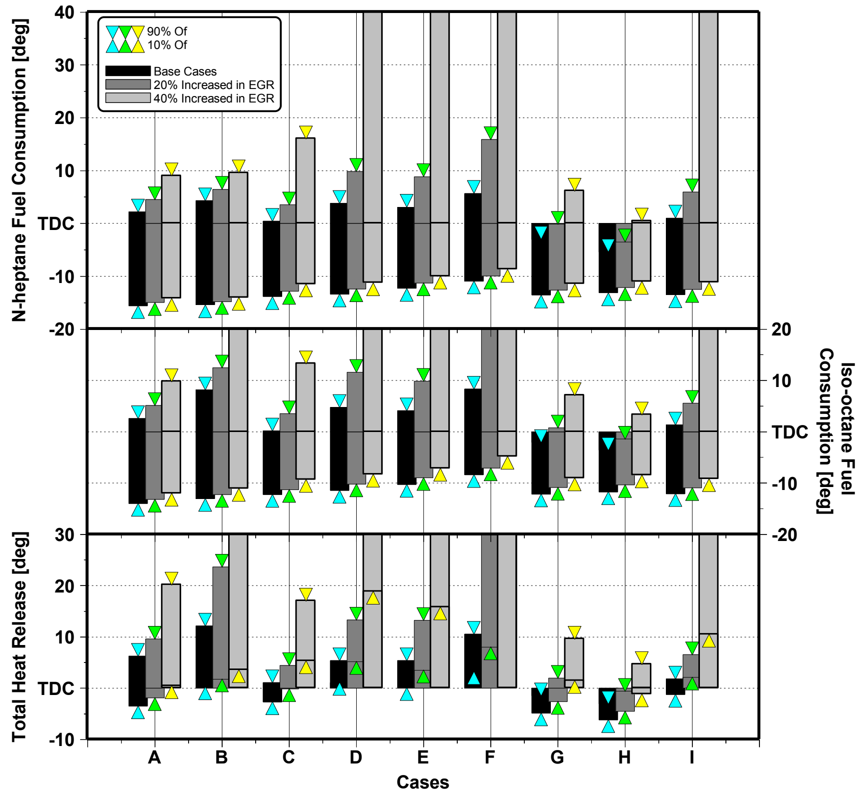

Fig. 13. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the cases with increasing in EGR without increasing boost pressure.

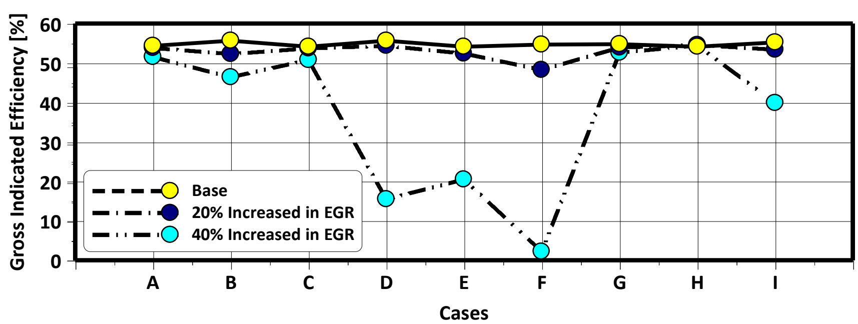

Fig. 14. Gross indicated efficiency in the cases with increasing in EGR without increasing boost pressure.

noted cases are in lean conditions, increasing the EGR level under the above-mentioned circumstance with the notable amount of excess air, increases the concentration of oxygen as well as H_2O and CO_2 in a perfect combustion.

Previously the reduction of equivalence ratio was considered with regard to increasing oxygen concentration, where it was increased by 17% and 42%, separately. While 20% and 40% of exhaust gasses were recirculated into the cylinder, the mass of intake air increased by 14% and 48%, respectively. So from the viewpoint of intake air mass, a 15% reduction in equivalence ratio can be quite comparable to a 20% enhancement in EGR level.

Fig. 15 shows the results of n-heptane and iso-octane fuels consumption and also total heat released. As mentioned about the reduction of equivalence ratio, enhancing the intake air mass causes the advance in the start of combustion. But in a case of using EGR, a longer combustion phase can be achieved which can improve the engine performances in cases such as C, D, E and I as shown in Fig. 15. However, in cases such as G and H in which the injection is retarded to near TDC, the EGR effect disappears due to the shortage of total heat release time. Also, EGR enhancement has strongly affected the cases with a relatively high amount of total fuel and n-heptane fuel so that a remarkable part of the fuel stays unburnt and leaves the cylinder.

Fig. 16 shows the effects of the increase in EGR rate on NO_x emission. Except for cases G and H, the NO_x level is even less than EPA 2010 standard which implies the effectiveness of EGR in the cases with proper combustion duration.

3.2.3. *The effects of increase in n-heptane fuel injection pressure*

To investigate the effects of increasing the injection pressure, two set of injection pressure 1100 bar and 1400 bar were selected. As shown in Fig. 17, increasing the injection pressure enlarges the spray penetration length and therefore the injection duration gets shortened to keep the amount of total fuel mass constant. This can accelerate the n-heptane fuel evaporation process as well as the start of combustion. Consequently, the duration of total heat release

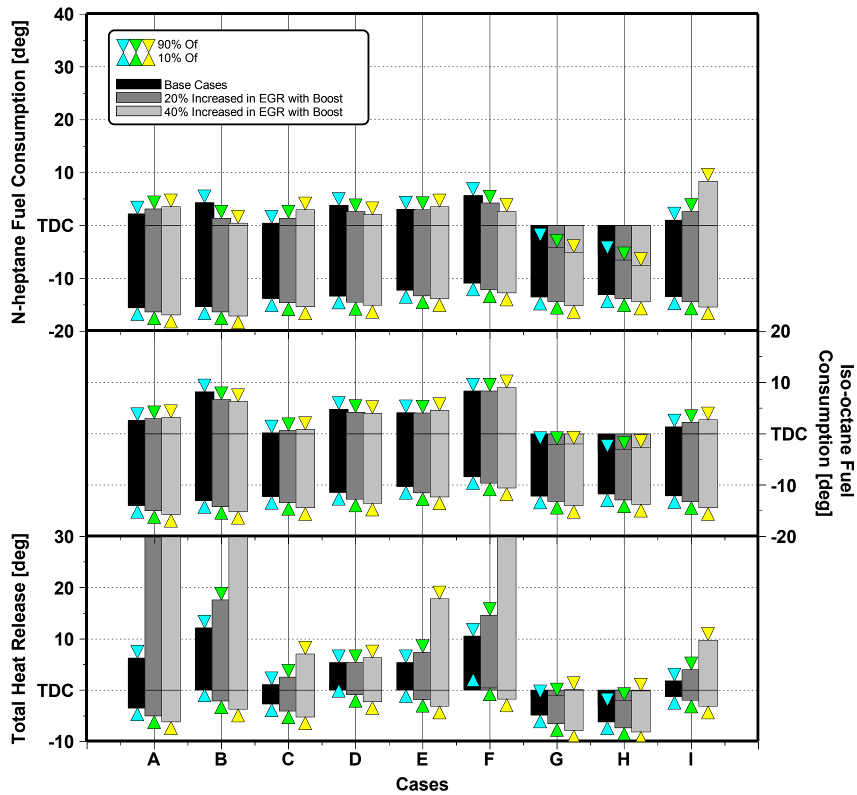

Fig. 15. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the cases with increasing in EGR with increasing boost pressure.

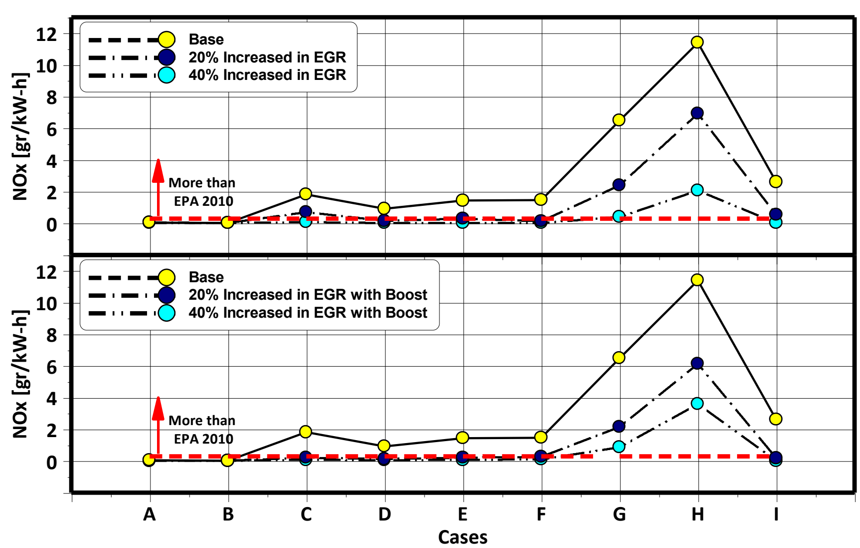

Fig. 16. NO_x production in the cases with increasing in EGR with and without boost pressure.

was found to get slightly shortened in most cases.

As depicted in Fig. 18, the amount of NO_x emission has stayed unchanged in cases A, B, D, E, and F. However in cases G, H, and I, contrary to case C, NO_x is less produced due to in-cylinder temperature reduction.

3.2.4. Using EGR and ethanol fuel with increase in compression ratio

In this section, the effects of a combination of different parameters on combustion process were investigated. Increasing the amount of ethanol fuel by itself can make longer delay on the start of combustion due to enhancing primary fuel octane number. Further increase in ethanol fuel leads to incomplete combustions. Also Increasing compression ratio has been proved to cause an advance in combustion phase since the diesel-type fuel reaches to the auto-ignition temperature much earlier than before. Although a higher compression ratio can increase thermal efficiency and improves performance in a sense via inhibiting an incomplete combustion, but in RCCI engines, the only augmentation in compression ratio has not overall positive effects on engine performance;

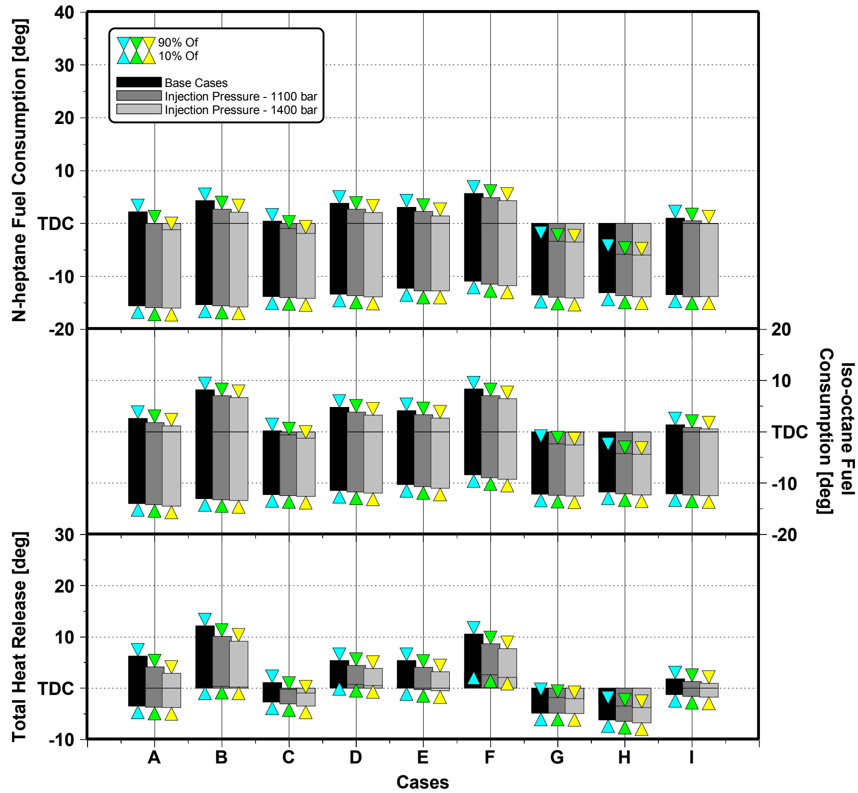

Fig. 17. The start and duration of n-heptane and iso-octane fuels consumption and total heat release in the cases for increasing injection pressure.

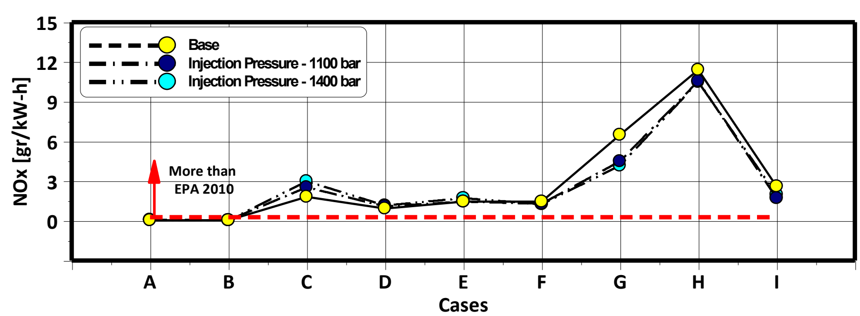

Fig. 18. NO_x production in the cases with increasing injection pressure.

especially about the cases which suffer from near-TDC instantaneous combustion. Similarly adding ethanol fuel to the gasoline-type fuel cannot be suitable due to incomplete combustion. Hence, both parameters have been applied to the engine to investigate their overall effect on combustion and emission of all cases. Accordingly, the compression ratio is increased by 1.4 as well as 20% of iso-octane fuel is replaced by ethanol.

In the next step, the effects of increasing both EGR and compression ratio were investigated. As shown in Fig. 13, increasing EGR without increasing boost pressure prolonged combustion duration and also combustion delay. However, in some cases, EGR caused an incomplete combustion as combustion efficiency reduced to below 90%. Hence in the second step, the simulation was conducted under the condition of increasing the compression ratio to 17.5 and the EGR rate by 40% without changes in boost pressure. The results are demonstrated in Fig. 19.

As it is clear in Fig. 19, adding ethanol fuel in case A was effective in retardation of combustion phase but on the negative side, it deteriorated combustion efficiency in case B where about 20% of total fuel remained unburned. This is why the duration of combustion from 10% to 90% of fuel consumption is very long. In other cases, the situation was not affected so much and the engine performance was slightly improved. Increasing EGR rate and the compression ratio was also beneficial in all cases except for case F. Although the implemented conditions slightly improved the situation in cases H and G, but it is still expected in these cases to have a spontaneous heat release and extreme ringing intensity due to pushing fuel injection to near TDC.

Results for NO_x production under mentioned conditions are depicted in Fig. 20 in which the effects of both conditions on NO_x reduction can be easily compared. As it is obvious, increasing EGR rate can decrease NO_x more effective than adding ethanol fuel in the way that the predicted amounts for produced NO_x are under EPA 2010 limit in most cases with using EGR.

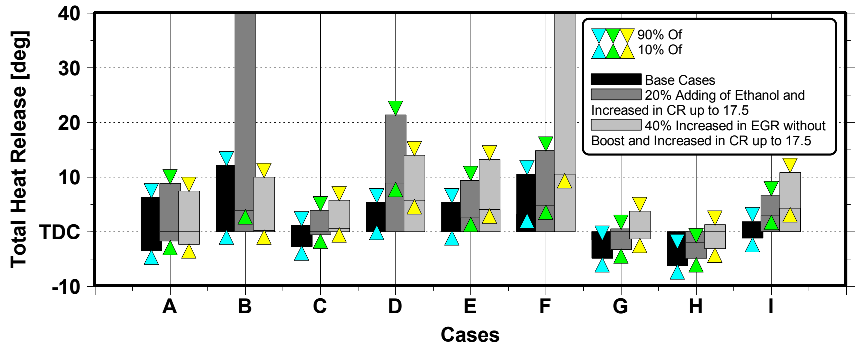

Fig. 19. Total heat release in the cases with combination of different parameters.

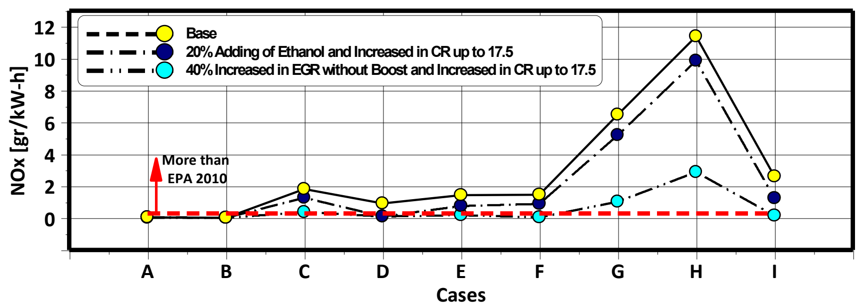

Fig. 20. NO_x production in the cases with combination of different parameters.

4. Conclusion

In the present study, major influential parameters on the start of combustion and combustion duration of an RCCI engine were studied in detail and extensively for all different possible scenarios. The RCCI engine performance and emissions are evaluated by means of the developed computational model which is well validated by experimental data (Kokjohn et al., 2011; Splitter, 2010). Some of the main findings are listed as following:

1 The equivalence ratio was changed using different boost pressure. Making the mixture lean by enhancing the oxygen concentration within the cylinder causes a shorter spray penetration length and earlier low and high-temperature reactions which advance the combustion phase. In addition to some improvements in some cases, a higher oxygen concentration also reduces the combustion temperature and consequently NO_x production. It was also perceived that increased equivalence ratio is more effective in cases with higher speed and higher amount of iso-octane fuel from combustion duration, ringing intensity and NO_x reduction point of view. The lean mixture was found to be effective only in the case with the low amount of total fuel and only when the mixture is highly diluted.

2 The EGR effects are looked for different cases where it superseded a part of fresh intake air to the cylinder also when boost pressure was used to maintain the primary amounts of intake air. Since the recirculated gasses can prolong the combustion duration, can improve the cases with unfavorable performing conditions. However, implementing high levels of EGR with regard to whether boost pressure is increased or not, can have different outcomes. While a level of 20% EGR without enhanced boost pressure was applied, an improvement in performance and NO_x emission of most of the cases was found. The exception was for the case in which the injection time was near TDC and case in which the engine speed was as high as 2100 rpm. Further increases in EGR rate caused penalties in efficiency and incomplete combustion. Using 20% and 40% EGR with enhanced boost pressure had positive effects on case B and on cases with high speed but negligible effects on the other cases.

3 The increase in injection pressure reduced NO_x emission slightly especially in cases with injection near TDC, increasing injection pressure was not seen to have any noticeable effect on prolonging combustion duration and on improving engine performance.

4 The effects of combined different parameters were investigated. At first, the compression ratio was augmented by 1.4 and 20% of iso-octane fuel was replaced by ethanol fuel as a fuel with high octane number, and in the second combination, 40% of the intake air was replaced by recirculated exhaust gasses and the compression ratio was augmented by 1.4. Both conditions were found to be effective in prolonging combustion duration and engine performance as well as, abating NO_x emission in almost all cases but EGR role in NO_x reduction was observed to be more significant.

Combustion in RCCI engines which is controlled by changes in amounts of two fuels with different reactivity has been able to improve combustion and performance in HCCI engines. For this purpose, reaching to a comprehensive intuition of all influential parameters on combustion duration and initiation can be essential for further developments of these engines.

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